

Lattice orientation and crack size effect on the mechanical properties of Graphene

P. R. Budarapu · B. Javvaji · V. K. Sutrarakar ·
D. Roy Mahapatra · M. Paggi · G. Zi · T. Rabczuk

Received: 26 January 2016 / Accepted: 11 April 2016
© Springer Science+Business Media Dordrecht 2016

Abstract The effect of lattice orientation and crack length on the mechanical properties of Graphene are studied based on molecular dynamics simulations. Bond breaking and crack initiation in an initial edge crack model with 13 different crack lengths, in 10 different lattice orientations of Graphene are examined. In all the lattice orientations, three recurrent fracture patterns are reported. The influence of the lattice orientation and crack length on yield stress and yield strain of Graphene is also investigated. The arm-chair fracture pattern is observed to possess the lowest yield properties. A sudden decrease in yield stress and yield strain can be noticed for crack sizes <10nm. However, for

larger crack sizes, a linear decrease in yield stress is observed, whereas a constant yield strain of ≈ 0.05 is noticed. Therefore, the yield strain of ≈ 0.05 can be considered as a critical strain value below which Graphene does not show failure. This information can be utilized as a lower bound for the design of nano-devices for various strain sensor applications. Furthermore, the yield data will be useful while developing the Graphene coating on Silicon surface in order to enhance the mechanical and electrical characteristics of solar cells and to arrest the growth of micro-cracks in Silicon cells.

Keywords Graphene fracture · Molecular dynamics · Bond elongation and rotation · Lattice orientation and initial crack size

P. R. Budarapu (✉) · M. Paggi
IMT School for Advanced Studies Lucca, Piazza San
Francisco 19, 55100 Lucca, Italy
e-mail: pattabhi.budarapu@imtlucca.it

B. Javvaji · D. Roy Mahapatra
Department of Aerospace Engineering, Indian Institute of
Science, Bangalore 560012, India

V. K. Sutrarakar
Aeronautical Development Agency, Defence Research and
Development Organization, Bangalore 560017, India

G. Zi · T. Rabczuk
School of Civil, Environmental and Architectural
Engineering, Korea University, Seoul 136-701, Korea

T. Rabczuk
Institute of Structural Mechanics, Bauhaus University of
Weimar, 99423 Weimar, Germany

1 Introduction

Graphene, an ultimately thin monolayer of carbon atoms packed into a hexagonal lattice, is the basic building block for graphitic materials of all other dimensionalities (Geim 2009; Huhu et al. 2014; Morpurgo 2015; Ying-Yan et al. 2014). Because of its several useful material properties (Changgu et al. 2008; Fengnian et al. 2014; Fiori et al. 2014; Kravets et al. 2014; Mics et al. 2015; Sarma et al. 2011; Schwierz 2010; Weiwei et al. 2015), Graphene finds wide range of applications (Budarapu et al. 2009, 2014c; Kinam et al. 2011; Kostarelos and Novoselov 2014; Liu 2014; Pospischil et al. 2014; Quan et al. 2015; Rodrigues et al. 2015; San-

tanu et al. 2012; Son et al. 2015; Traversi et al. 2014; Wen et al. 2012; Xue et al. 2014; Xuechao et al. 2015; Zhang et al. 2013). It can also be used as a strengthening component in composites (Chen et al. 2015a; Kim et al. 2013; Shin et al. 2015; Zan et al. 2015). As the demand for Graphene-based applications is growing, it is important to deeply understand its mechanical and challenging failure characteristics. Chuvilin et al. (2009) studied the growth of two holes created by radiation in Graphene nano ribbons, based on the imaging side spherical aberration-corrected transmission electron microscopy at 80kV. As the holes grow and two holes approach each other, they observed the transitions and deviations from the hexagonal structure involving some reconstructions resulting into more pentagons and heptagons than hexagons, which turned out to be stable. Jin et al. (2009) explained the structural dynamics of carbon atomic chains such as formation, migration, and breakage observed in the experiments, by density-functional theory calculations. However, estimating the mechanical properties of Graphene is challenging due to the practical difficulties in setting-up experiments (Kim et al. 2012). Hence, numerical simulations are good alternatives for predicting fracture related properties. Several researchers have investigated the mechanical properties of Graphene based on molecular dynamics simulations (Chen et al. 2015b; Gamboa et al. 2015; Grantab et al. 2010; Hadden et al. 2015; Pei et al. 2010; Tiwary et al. 2015a,b; Vadukumpully et al. 2011).

Bu et al. (2009) investigated the mechanical behavior of Graphene nanoribbons based on Tersoff potential function. They reported the increase in the Young's modulus due to stress stiffening, when the strain exceeds 18%. Peng et al. (2014) have measured the fracture toughness of Graphene based on experiments, validated with numerical simulations. They also verified the applicability of the classic Griffith theory of brittle fracture to Graphene. They observed that the critical stress intensity factor (K_{IC}) is not constant when the initial crack length is less than a certain value. Ansari et al. (2012) have studied the presence of vacancy defects in Graphene based on the Tersoff–Brenner potential function and reported significant reduction in the ultimate strength in the zig-zag direction, while the effect is minimal on the Young's modulus. Khare et al. (2007) have studied the effects of large defects and cracks on the mechanical properties of carbon nanotubes and Graphene sheets using

the coupled quantum mechanical/molecular mechanical approach based on the Tersoff–Brenner potential. They observed that the weakening effects of holes, slits, and cracks will vary only moderately with the shape of the defect, and instead depend primarily on the cross-section of the defect perpendicular to the loading direction and on the structure near the fracture initiation point.

Jhon et al. (2012, 2014) estimated the anisotropic fracture response of Graphene based on molecular dynamics simulations. They found that both the tensile strength and strain remain almost constant up to an orientation angle of 12° . Then a rapid increase resulting in a remarkable degradation of the tensile strength compared to brittle fracture counterpart, was reported. They also noticed that fracture pattern holds in the range 100–700 K. Sun et al. (2015) investigated the orientational anisotropic effect on the fracture strength of vacancy-defective Graphene using molecular dynamics simulations. They concluded that the fracture strength of Graphene at the orientation angle of 15° has the smallest sensitivity to vacancy defects due to the minimization of stress concentration in that direction. Also, the fracture strength in the zig-zag direction was found to be more sensitive to the vacancy defects. Cao (2014) used the quantum mechanical and classical molecular dynamics simulations to understand the mechanical behavior of Graphene. However, the above studies were carried out on Graphene without initial cracks. Hence, the effect of lattice orientation on the crack growth dynamics was ignored.

Zhao et al. (2009) have investigated the mechanical strength and properties of Graphene under uniaxial tensile test as a function of size and chirality using the orthogonal tight-binding method and molecular dynamics simulations with an adaptive intermolecular reactive empirical bond order (AIREBO) potential. They reported reasonable agreement of their estimated results on Young's modulus, fracture strain and fracture strength of bulk Graphene, with the published experimental data (Changuu et al. 2008; Liu et al. 2007). They also observed that the Griffith criterion overestimates the strength of cracks shorter than 10 nm and hence used a strength based criterion to explain the yield behaviour.

Recently, Datta et al. (2015) have investigated:

1. The effect of two lattice orientations (arm-chair and zig-zag) with different crack lengths (for a/b ratios

137 upto 0.25) in mixed mode loading conditions at 300
 138 and 1000 K, while keeping the crack perpendicular
 139 to the orientations.

140 2. The effect of crack orientation in the arm-chair and
 141 zig-zag Graphene, retaining the same loading direc-
 142 tions.

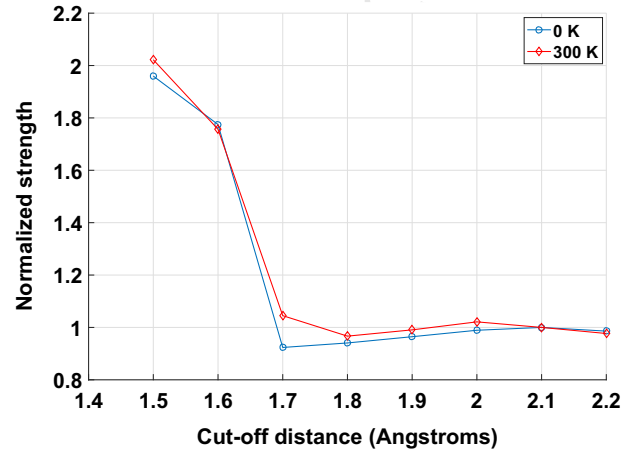
143 Their main objective is to study the fracture toughness,
 144 using the AIREBO potential function. In the present
 145 work, we study 10 different orientations with 13 differ-
 146 ent crack lengths. We always load Graphene along the
 147 direction perpendicular to the crack length to study the
 148 Mode I fracture. This is similar to the first case inves-
 149 tigated in [Datta et al. \(2015\)](#) for arm-chair and zig-zag
 150 Graphene. In the present work, our focus is mainly on
 151 estimating the mechanical properties of Graphene and
 152 the coupled effect of the lattice orientations and initial
 153 crack length on the mechanical properties, based on
 154 the Tersoff potential function. Therefore, the relations
 155 between the lattice orientation and the crack pattern and
 156 between the initial crack size and lattice orientation on
 157 the mechanical properties of Graphene are investigated.
 158 The final aim is to come up with a design criterion
 159 which can be used in the nano-devices for strain sensor
 160 applications.

161 The followings are the main objectives of the present
 162 study: (1) identification of limiting strain below which
 163 Graphene never fails; (2) combined effect of the lattice
 164 orientation and crack size on the mechanical properties
 165 of Graphene; (3) identification of fracture pattern for
 166 each given lattice orientation; and (4) the variation of
 167 the tensile strength with chiral angle. All the above
 168 results are important for the design of Graphene-based
 169 nano devices.

170 The arrangement of the article is as follows: Details
 171 of the numerical model are explained in Sect. 2. The
 172 effect of lattice orientation and crack size in the yield
 173 properties of Graphene are discussed in Sect. 3. The
 174 key findings are summarized in Sect. 4.

175 **2 Atomistic modelling and simulations**

176 In this work, the atom to atom interactions of carbon in
 177 Graphene are simulated based on the Tersoff potential
 178 (1989). Tersoff potential has been successfully applied
 179 to predict mechanical properties of Graphene ([Bu et al.](#)
 180 [2009](#); [Budarapu et al. 2015](#); [Thomas and Ajith 2014](#);
 181 [Volokh 2012](#)). The mathematical expression of the
 182 bond energy of the atomistic model based on the Tersoff



183 **Fig. 1** Variation of the normalized strength at the first bond
 184 break with cut-off distance at 0 and 300 K, with an initial crack
 185 length of 0.5L and when the lattice is oriented along 0°. The
 186 fracture strength at the first bond break is normalized with the
 187 corresponding value at $r_c = 2.1 \text{ \AA}$

188 potential can be expressed as ([Tersoff 1989](#)):

$$189 V(r_{\alpha\beta}) = f_c(r_{\alpha\beta})[f_R(r_{\alpha\beta}) + b_{\alpha\beta}f_A(r_{\alpha\beta})] \quad 194$$

$$195 f_R > f_c, \quad f_A > b_{\alpha\beta} \quad 196 \quad (1) \quad 197$$

198 where $r_{\alpha\beta}$ is the distance between the atoms α and β .
 199 The bond energy in the Tersoff framework is a combina-
 200 tion of attractive (f_A) and repulsive (f_R) energy
 201 functions, which are expressed in the form of the expo-
 202 nential Morse like functions; f_c is a smooth spherical
 203 cut-off function around atom α based upon the dis-
 204 tance to the first nearest neighbour cell. Details of the
 205 variables of potential function in Eq. (1) are explained
 206 in ‘‘Appendix’’. Variation of the normalized fracture
 207 strength with the effect of cut-off distance (r_c) at 0
 208 and 300 K are plotted in Fig. 1. In Fig. 1, the fracture
 209 strength at the first bond break is normalized with the
 210 corresponding value at $r_c = 2.1 \text{ \AA}$. According to Fig. 1
 211 and to ([Shenderova et al. 2000](#); [Zhao and Aluru 2010](#)),
 a cut-off distance of 2.1 \AA is considered to reproduce
 the physical observations, even at higher temperatures.
 Hence, $r_c = 2.1 \text{ \AA}$ is used in all the simulations of the
 present work.

The main aim of the present work is to understand
 the effect of lattice orientation on the crack initia-
 tion and growth mechanics and hence, on the mechan-
 ical properties of Graphene. To achieve this objec-
 tive, an uni-axial tensile deformation test of Graphene
 is studied with varying lattice orientation and initial
 crack length (a_0). Ten different lattice orientations of
 Graphene are characterized by the following chiral vec-

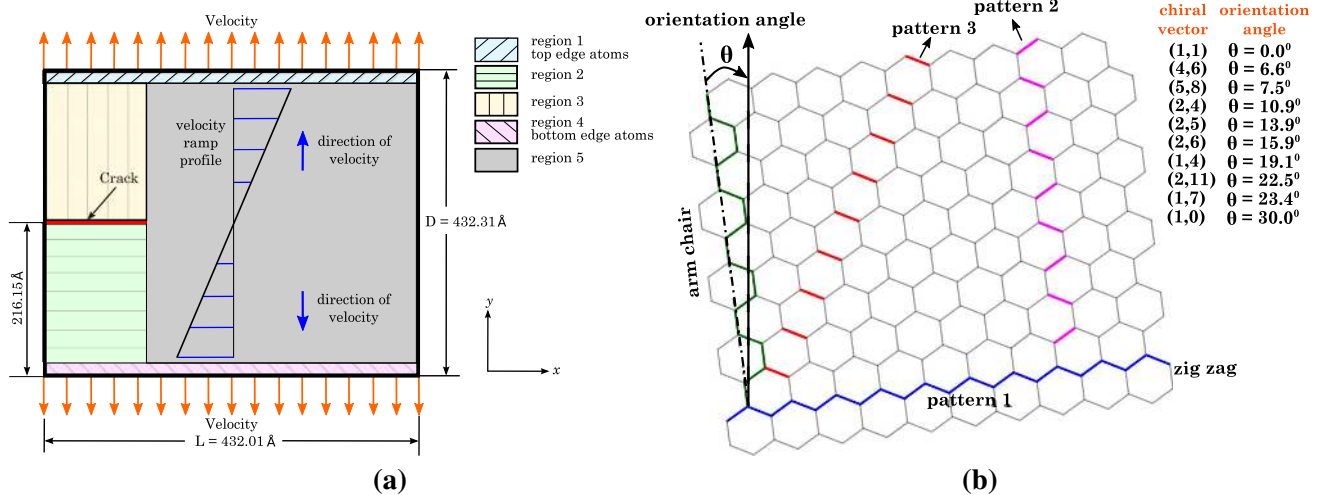


Fig. 2 **a** Schematic of the edge crack model used in all the examples and **b** schematic showing the observed three fracture patterns along with the orientation angle, arm-chair and zig-zag directions

tors: (1,0), (1,1), (4,6), (5,8), (2,4), (2,5), (2,6), (1,4) (2,11), (1,7). Thirteen different initial crack lengths are also considered, namely: 0.025L, 0.05L, 0.1L, 0.15L, 0.2L, 0.25L, 0.33L, 0.4L, 0.5L, 0.6L, 0.7L, 0.8L, and 0.9L, where L is the width of the sample, see Fig. 2.

The hexagonal lattice structure of the Graphene sheet with a lattice constant 2.45 \AA , is considered to develop the atomistic model. An initial edge crack is created in the middle of the vertical side. The lattice domain has overall dimensions of 432.01 \AA (L) \times 432.31 \AA (D), as shown in Fig. 2a. The corresponding full scale atomistic model consists of a set of atoms ranging from 74,880 to 75,269, depending on the lattice orientation angle. To model the crack, the total domain is partitioned into several regions, see Fig. 2a. Atoms on the top and bottom edges of the domain belong to regions 1 and 4, respectively. The crack in the atomistic model is identified based on the distance between two neighboring atoms. However, the initial crack in the atomistic model is created by restricting the interactions between the set of atoms on either side of the crack surface, which is achieved by updating the neighbour list accordingly. The degrees of freedom along the x-direction of the left and right edge atoms and along the y-direction of the top and bottom edge atoms, are restrained. An initial velocity of 0.1 angstroms/pico-seconds ($\text{\AA}/\text{ps}$) along the y-direction is prescribed on the top and bottom edge atoms. A ramp velocity profile as shown in Fig. 2a is adopted for the rest of the domain. All the simulations in the present work are carried out using the open source Large-

scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software (Plimpton 1995).

In the present work, a ‘load cycle’ is defined as prescribing the velocity on the top and bottom edge atoms for a specified time period, followed by an equilibration for another specified time period. In each load cycle, the prescribed velocity on the top and bottom edge atoms is applied for another period of 1 ps, after which the system is equilibrated for a period of 1 ps. The computed stress is the averaged stress estimated based on the Virial theorem (Marc and McMillan 1985; Subramaniyan and Sun 2008). The average virial stress (σ) over a volume Ω with total number of atoms n^A is calculated as

$$\sigma = \frac{1}{\Omega} \left(\frac{1}{2} \sum_{\alpha=1}^{n^A} \sum_{\substack{\beta=1, \\ \beta \neq \alpha}}^{n^A} \mathbf{r}_{\alpha\beta} \otimes \mathbf{f}_{\alpha\beta} - \sum_{\alpha=1}^{n^A} m_{\alpha} \dot{\mathbf{u}}_{\alpha} \otimes \dot{\mathbf{u}}_{\alpha} \right) \quad (2)$$

where m_{α} is the mass of atom α , \mathbf{r} is the position vector, \mathbf{f} is the force vector and \mathbf{u}_{α} , $\dot{\mathbf{u}}_{\alpha}$ are the displacement and velocity vectors of atom α , respectively. The definition of Virial stress involves the instantaneous velocities only due to thermal fluctuation. Therefore, the Virial stress calculated from molecular dynamics simulations has to be time averaged in order to arrive at the equivalent continuum Cauchy stress. In this work, Virial stress is averaged over 500 time steps. Engineering strain is used as a measure of deformation, which is defined as $(l - l_0)/l_0$, where l is the instantaneous length of the

vertical side and l_0 is its initial value obtained after the first step of energy minimization corresponding to the initial configuration. The time integration of the equations of motion is carried out based on the Verlet algorithm (Swope et al. 1982). The effect of numerical stability has been investigated in Budarapu et al. (2015). Budarapu et al. (2015) have reported that 1.0 fs is sufficient to study the mechanical behavior of Graphene up to yielding. However, a much smaller time step is required to predict the crack growth more accurately. Since the objective is to study the yield properties, a time step of 1.0 fs has been considered in the present work.

All the simulations are performed under isothermal loading conditions, at a temperature of ≈ 0 K (0.1 K). In the isothermal loading, the system temperature is maintained constant. However, the application of the initial velocities would lead to increase in the kinetic energy and hence, the system temperature. Therefore, the isothermal conditions in the present work are achieved by velocity rescaling technique, where the velocities at each time step are rescaled to maintain the constant temperature of ≈ 0 K. The temperature of ≈ 0 K is considered to avoid the influence of temperature on the lattice orientations and crack length in the mechanical behavior of Graphene. Furthermore, to observe the trends in mechanical properties with temperature, some simulations are carried out at 300 K. The stress–strain curves at ≈ 0 K are compared to the results at 300 K, as explained in the results and discussion Sect. 3. However, the complete study of the effect of temperature on the mechanical response by varying lattice orientations and crack length is beyond the scope of the present work.

The maximum Cauchy stress for a uni-axial tensile test in the arm-chair and zig-zag direction is found to be 110 and 121 GPa (Liu et al. 2007; Zhao et al. 2009), respectively. The intrinsic breaking strength of perfect Graphene is reported as 130 ± 10 GPa (Changgu et al. 2008; Zhao et al. 2009). Depending on the size of the defect, the fracture stress of the defective Graphene varies from 30 to 120 GPa (Khare et al. 2007; Zhang et al. 2012b). However, the fracture stress is observed to drop sharply from 120 GPa, for small initial defect sizes and tend to 30–60 GPa, after a certain defect size. The ability of a material containing a crack to resist fracture is measured by its fracture toughness property. The critical stress intensity factor (Peng et al. 2014) denoted by $K_{IC} = \sigma_c \sqrt{\pi a_0}$, where σ_c is the critical stress of onset

of fracture and a_0 is the initial crack length, is conventionally used to characterize the fracture toughness of Graphene. As reported in Peng et al. (2014), the factor $\sigma_c \sqrt{a_0}$ remains constant irrespective of the initial crack length. Therefore, the fracture toughness of Graphene is expected to remain constant with respect to the size of the initial crack as well.

3 Results and discussions

3.1 Orientation dependent crack pattern

We performed the fracture simulations of 10 different lattice orientations with 13 different initial crack lengths, to estimate the yield properties corresponding to each combination of lattice orientation and initial crack length. The yield properties, namely the yield stress and yield strain are the stress and strain values captured at the time of first bond break. Based on the results, three different patterns of crack growth in Graphene as labeled in Fig. 2b are observed. The pattern labeled as 1 is observed in the arm-chair Graphene (0°). A similar pattern is also observed in the 6.6° , and 10.9° orientations. The second pattern is noticed only in the zig-zag Graphene, oriented at 30° . Whereas, the third pattern is observed when the Graphene is oriented along the remaining six orientations, namely: 7.5° , 13.9° , 15.9° , 19.1° , 22.5° , and 23.4° . Therefore, we specifically select 0° , 13.9° , and 30° orientations to understand the crack growth patterns and hence the variation of the associated mechanical properties.

The initial atomic configuration at 0° orientation is shown in Fig. 3a. Atoms around the crack tip are marked with labels 'A' to 'P', where the color of the atoms indicates their potential energy. A portion of the atoms around the crack tip for the 0° , 13.9° and 30° lattice orientations is also shown in Figs. 4a, 5a and 6a, respectively. In the initial configuration, all the atoms are assumed to have the same potential energy. The initial crack is created by deleting the bonds between the atoms and updating the neighbour list accordingly. The dashed lines in Figs. 4a, 5a and 6a shows the deleted bonds and hence the size of the initial crack. A strain load is prescribed on a group of atoms along the top and bottom surfaces of the lattice, as shown in Fig. 2a. Therefore, based on the given loading and boundary conditions, the bond D–C is the first loaded bond. Con-

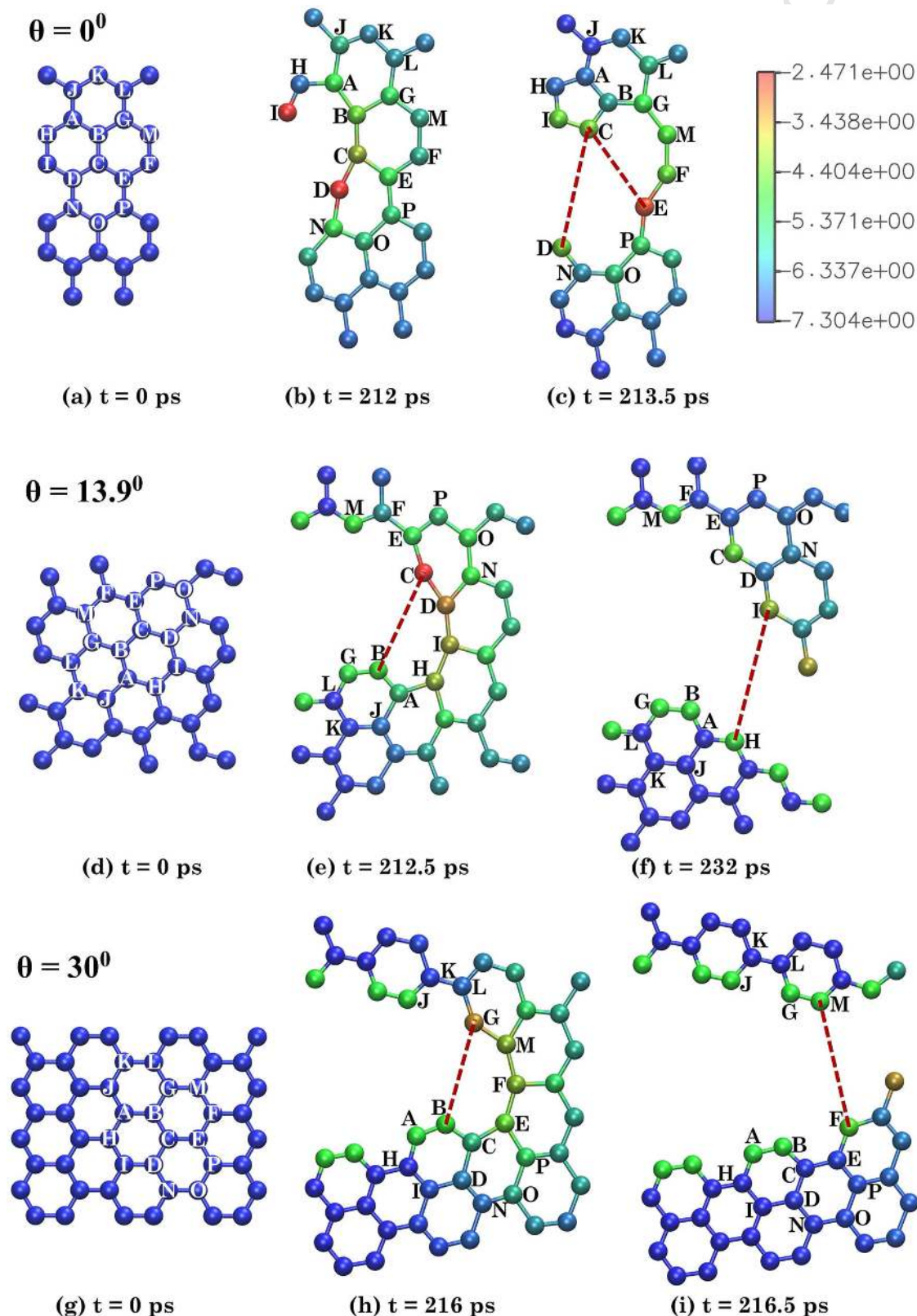


Fig. 3 Atomic configurations around the crack tip in the initial and during the first and second bond break, when the Graphene lattice is oriented along 0° , 13.9° and 30° , in the *top*, *middle* and *bottom* rows respectively. The *dashed lines* indicate the broken bonds

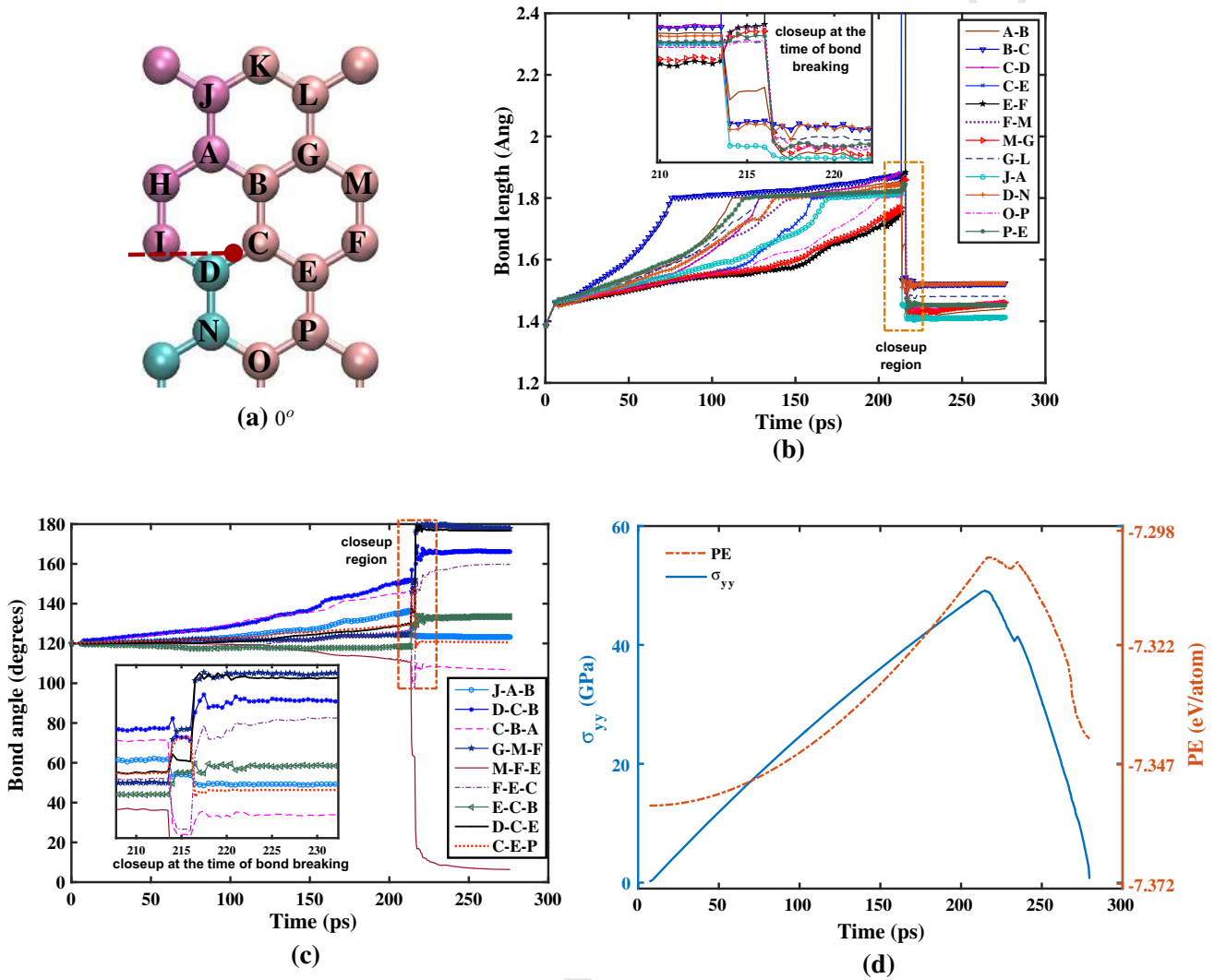


Fig. 4 a Atom position in the initial configuration when the lattice is oriented along the 0° , along with the atoms around the crack tip. Variation of the **b** bond length, **c** bond angles and **d**

strain along the y direction and the potential energy per atom, with time. The pictures in the bottom of **c** shows a closeup at the time of bond breaking. Plot **d** is generated for $a_0 = 0.5L$

364 tinuous increase loading leads to stretching of the bonds
 365 connecting the atoms D–C–E. When the bond length
 366 reaches a certain threshold, the bond between D–C
 367 breaks first at 213 ps, further transferring the load to
 368 the next symmetric bond C–E, which finally breaks at
 369 213.5 ps as shown in Fig. 3c. The load transfer is con-
 370 firmed by the shifting of the higher energy from atom D
 371 to atom E, refer to Fig. 3a–c. The next bond to break is
 372 E–F. Remaining bonds like A–B, B–G, D–N and N–O
 373 are found to be stable with equilibrium bond length.

374 The initial configuration with the lattice oriented
 375 along the 13.9° is shown in Fig. 3d. In this orienta-
 376 tion, the bond B–C is observed to be the first loaded,

377 which breaks at 212.5 ps as indicated in Fig. 3e. After
 378 the failure of the bond, the load is observed to be
 379 transferred to atom I from atom C through atom D.
 380 This leads to the failure of bond I–H at 232 ps, see
 381 Fig. 3f.

382 The initial configuration when the lattice is oriented
 383 along 30° , is shown in Fig. 3g. In this configuration,
 384 the bond connecting atoms G–B is observed to break
 385 first at 216 ps, followed by the failure of the symmetric
 386 bond M–F at 216.5 ps, refer to Fig. 3h, i.

387 Initial configurations of the lattice oriented along 0° ,
 388 13.9° and 30° are shown in Figs. 4a, 5a and 6a, respec-
 389 tively. Stretching of various bonds with time in the 0°

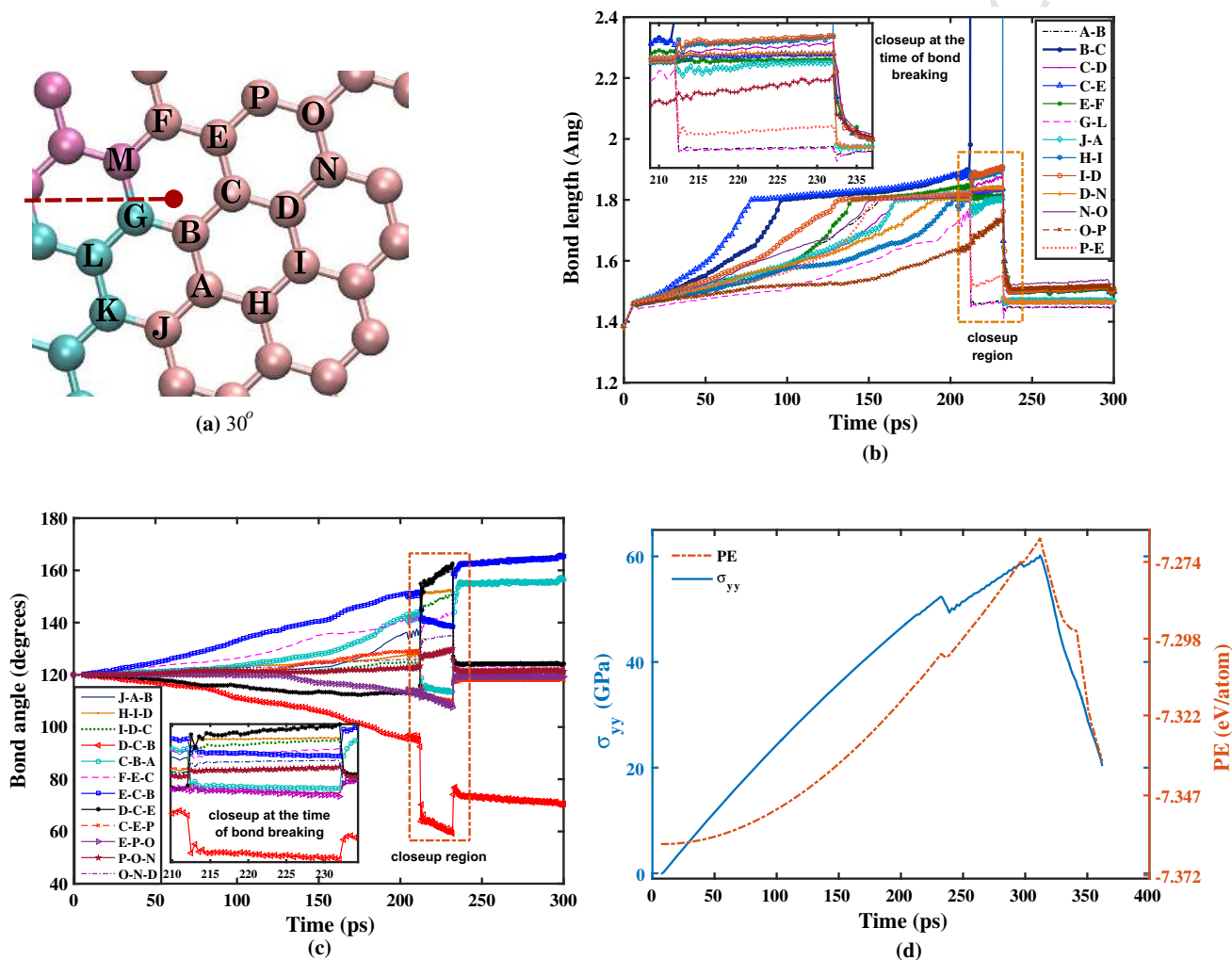


Fig. 5 **a** Atom position in the initial configuration when the lattice is oriented along the 13.9° , along with the atoms around the crack tip. Variation of the **b** bond length, **c** bond angles and **d**

strain along the y direction and the potential energy per atom, with time. The pictures in the bottom of **c** shows a closeup at the time of bond breaking. Plot **d** is generated for $a_0 = 0.5L$

orientation is plotted in Fig. 4b, where the picture on the top shows a closeup of the selected region. It can be seen that the bond B–C starts initially to elongate, to reach a bond length of 1.8 \AA . Subsequently, the nearby bonds also start elongating, to reach the bond length of $\approx 1.8 \text{ \AA}$. When all the bonds around the crack tip reach the critical bond length, the bond C–D breaks first to create the first fracture. Results indicate that the bond length is the critical parameter to estimate fracture in Graphene. The corresponding change of bond angles with time are plotted in Fig. 4c. However, the bond rotation plotted in Fig. 4c cannot be considered as a parameter to estimate the bond breaking in Graphene. This is due to the following reasons: (i) oscillations in the bond angle until the first bond break; (ii) the bond

angles of the bonds around the crack tip change significantly due to reorientation of the bonds after the first bond break. Therefore, bond length can be considered as a parameter to predict the bond break in Graphene.

A similar trend and mechanical behaviour in bond stretching is observed when the lattice is oriented along the 13.9° and 30° , see Figs. 5b and 6b, respectively. The bonds around the crack tip started to stretch first, to reach a critical value. When all the bonds around the crack tip reach the critical value, failure takes place. The bond angles also follow a similar trend, but they cannot be considered as a parameter to predict the fracture for the reasons explained above. Variation of the stress in the loading direction (σ_{yy}) and the potential energy per

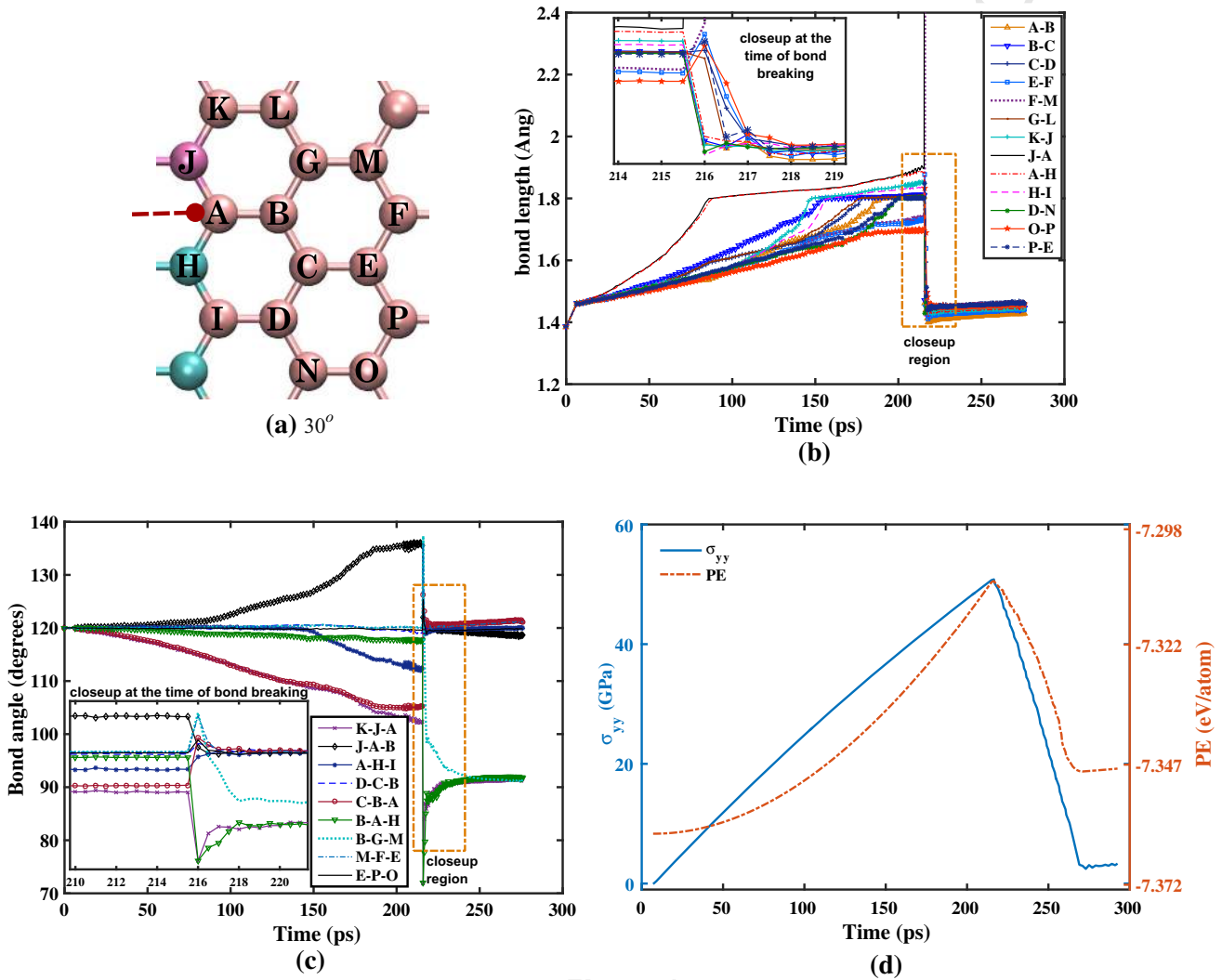


Fig. 6 a Atom position in the initial configuration when the lattice is oriented along the 30° , along with the atoms around the crack tip. Variation of the **b** bond length, **c** bond angles and **d**

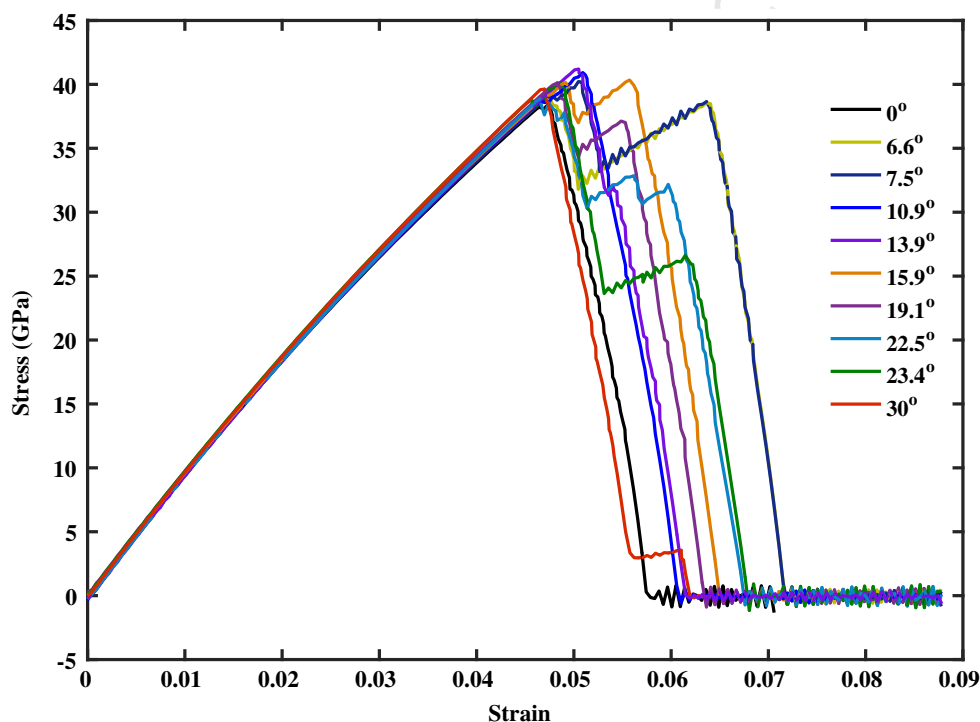
strain along the y direction and the potential energy per atom, with time. The pictures in the bottom in (c) shows a closeup at the time of bond breaking. Plot **d** is generated for $a_0 = 0.5L$

420 atom with time, when the lattice is oriented along 0° ,
 421 13.9° and 30° , is plotted in Figs. 4d, 5d and 6d, respec-
 422 tively. The first drop in stress as well as potential energy
 423 is considered for the estimation of the yield stress and
 424 yield strain of the materials. Based on Fig. 5d, it is inter-
 425 esting to note that the 13.9° lattice orientation shows a
 426 continuous increase in stress as well as potential energy
 427 even after the first bond break which is observed at
 428 213.5 ps, refer to the closeup of Fig. 5b. The increase
 429 in stress as well as potential energy is continued till
 430 the second bond breaks at 232.5 ps. Therefore, results
 431 indicate that special orientations of Graphene can lead
 432 to improvement in the mechanical properties even after
 433 first bond failure.

3.2 Lattice orientation dependent mechanical properties

436 In order to understand the effect of lattice orientation on
 437 mechanical properties of Graphene, the tensile stress–
 438 strain curves have been generated for all the 10 different
 439 orientations considered in the present work. Variation
 440 of the stress with strain, for different lattice orienta-
 441 tions is plotted in Fig. 7. Based on Fig. 7, it is observed
 442 that at zero strain all the orientations of Graphene have
 443 zero stress, which indicates that no residual stress exist
 444 in any of the configurations. Further strain controlled
 445 loading leads to continuous increase in strain which
 446 correspondingly leads to increase in stress. Due to the

Fig. 7 Stress–strain plots of all the ten different configurations considered in the present work



447 increase in strain, the bond length of an initial relaxed
 448 Graphene starts to increase. The atoms around the crack
 449 tip possess the highest potential energy. As soon as the
 450 bond lengths of the atoms around the crack tip reaches
 451 a critical value, the breaking of first bond occurs, indi-
 452 cated by a drop in the stress, leading to the yielding of
 453 Graphene. The corresponding stress and strain values
 454 are designated as yield stress and yield strain, respec-
 455 tively. Fluctuations in the yield properties of Graphene
 456 for different lattice orientations are observed. In order
 457 to study the effect of lattice orientation on yielding,
 458 yield stress and strain are plotted with lattice orienta-
 459 tions in Fig. 8.

460 Figure 8a, b shows the distribution of normalized
 461 yield stress and normalized yield strain with vary-
 462 ing lattice orientations from 0° (arm-chair) to 30°
 463 (zig-zag), respectively. The normalization is based on
 464 the yield values at 0°. The arm-chair Graphene is
 465 observed to possess the lowest yield stress, which
 466 further increases with increase in lattice orientation
 467 angle and reaches a maximum at 13.9°. Subsequent
 468 increase in lattice orientation leads to the reduction in
 469 yield stress until 22.5°. The yield stress is observed
 470 to increase with the lattice orientation until 30°. From
 471 Fig. 8a, the zig-zag configuration is observed to pos-
 472 sess a higher yield stress as compared to the arm-
 473 chair Graphene. Also a similar trend in yield strain is

474 observed. From Fig. 8b, it can be noticed that the arm-
 475 chair Graphene has a lower yield strain as compared to
 476 the zig-zag configuration. Yield strain also shows
 477 an increase in value by increasing lattice orientation
 478 and reaches maximum at 13.9°. Subsequent increase
 479 in lattice orientation leads to a drop in yield strain
 480 until 23.4°. Later on, the yield strain is observed to increase
 481 until 30°.

482 The state of equilibrium energy of an atomistic sys-
 483 tem depends on the arrangement of atoms in that partic-
 484 ular configuration. The structure will be stable when the
 485 system potential energy is minimum. In Graphene, the
 486 bonds along the loading direction will undergo more
 487 deformation and are responsible for failure with very
 488 similar bond elongation at the fracture point (Zhao et al.
 489 2009). Furthermore, the magnitude of the bond length
 490 and bond angle variation in the zig-zag direction is
 491 reported to be much larger than that of the arm-chair
 492 direction (Zhao et al. 2009). This indicates that the
 493 zig-zag configuration is energetically more stable and
 494 absorbs more energy before fracture, as compared to the
 495 arm-chair configuration. In other words, the arrange-
 496 ment of atoms in the arm-chair Graphene leads to an
 497 energetically unstable configuration. In this work, we
 498 observed that the stability increases with lattice orienta-
 499 tion reaching the maximum at 13.9°. Therefore, the
 500 potential energy is observed to be the lowest when the

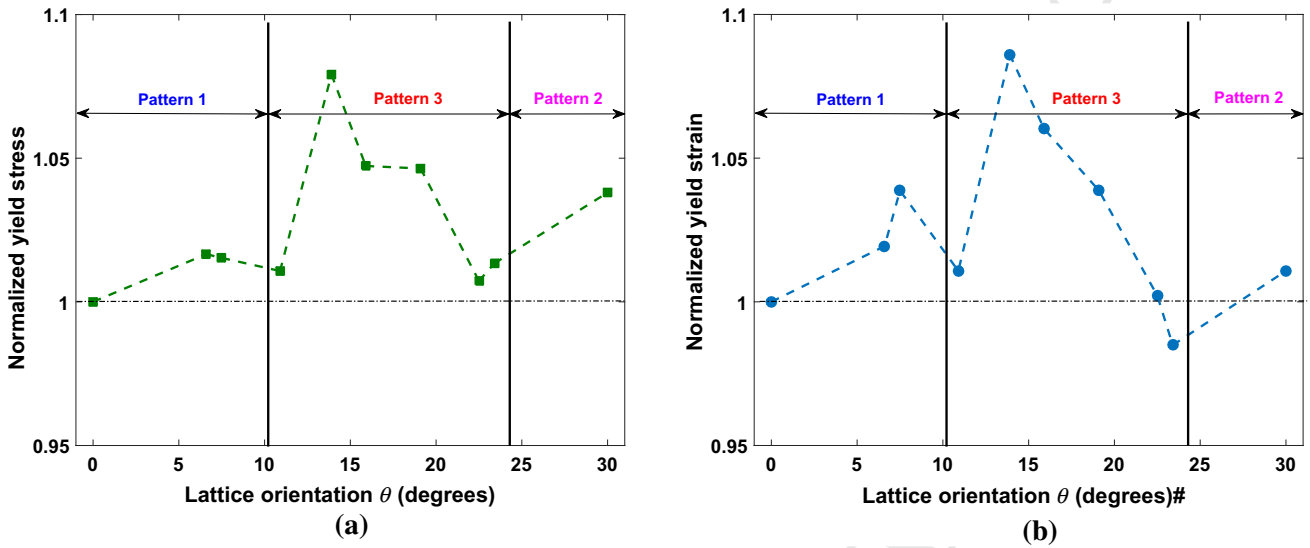


Fig. 8 Distribution of the **a** normalized stress and **b** normalized strain with the lattice orientation. The plots are generated based on the results with $a_0 = 0.5L$

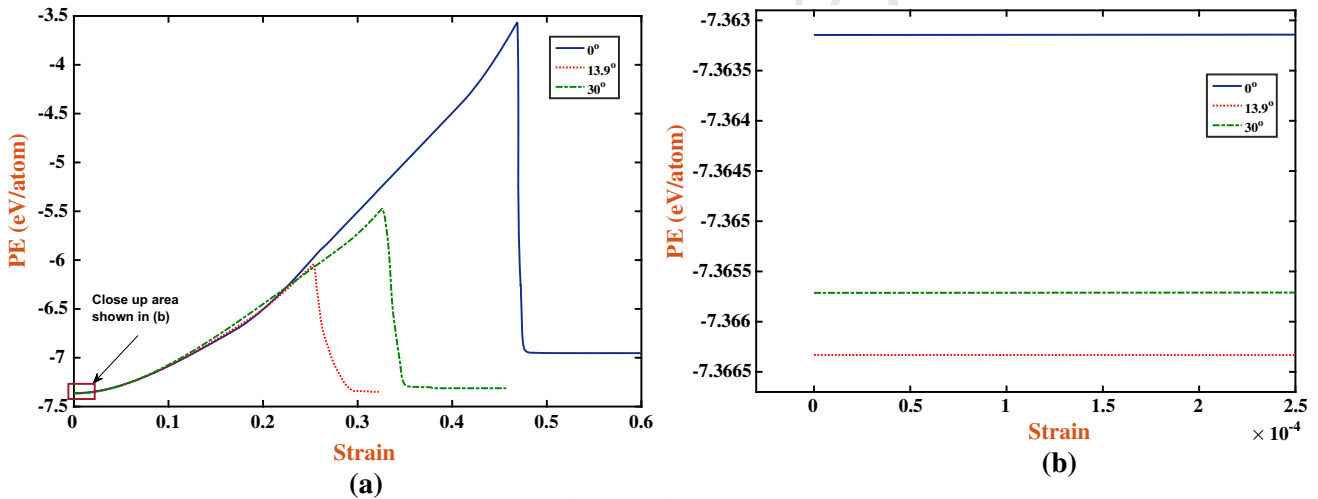


Fig. 9 Distribution of the **a** potential energy with strain and **b** a close up at the beginning, with zero strain. The plots are generated based on the initial potential energy of the system without any crack, after the minimization

501 lattice is oriented along 13.9° , as shown in Fig. 9. This
 502 explains the reasons for the highest potential energy of
 503 the arm-chair Graphene.

504 The lower fracture strength of arm-chair (0°)
 505 Graphene as compared to the zig-zag (30°) Graphene
 506 can be correlated to the system potential energy
 507 plotted in Fig. 9. Based on Fig. 9b, the arm-chair
 508 Graphene possesses the highest initial potential energy
 509 of -7.3631 eV/atom, as compared to other configura-
 510 tions considered in the present study. Due to the high-
 511 est initial potential energy of the arm-chair Graphene,
 512 an early yielding is anticipated. Whereas, the zig-zag
 513 Graphene is observed to possess an initial potential

energy of -7.3657 eV/atom, which is lower than the 514
 arm-chair Graphene. This indicates that the zig-zag 515
 configuration is more stable and hence it can sustain 516
 more strain, which leads to a higher fracture strength as 517
 compared to the arm-chair Graphene. Interestingly, the 518
 Graphene with chiral vector (2, 5) at 13.9° lattice 519
 orientation is found to be the most stable configuration 520
 with an initial potential energy of -7.3663 eV/atom, out of 521
 the 10 orientations considered in the present study. This 522
 is further confirmed by the highest fracture strength of 523
 Graphene when the lattice is oriented at 13.9° , refer to 524
 Fig. 8a. 525

526 Interestingly, the crack patterns discussed in Sect. 3.1
 527 for different lattice orientations can be correlated to the
 528 yield stress and yield strain values. The pattern num-
 529 ber 1 in Fig. 2b is observed in 0° (arm-chair), 6.6° ,
 530 and 10.9° configurations. However, pattern number 2 is
 531 observed only in 30° (zig-zag) orientation. The remain-
 532 ing lattice orientations (7.5° , 13.9° , 15.9° , 19.1° , 22.5° ,
 533 and 23.4°) are exhibiting the pattern number 3. In
 534 the first pattern, the crack initiation and growth takes
 535 place perpendicular to the loading direction, which cor-
 536 responds to the arm-chair (0°) configuration. Similar
 537 crack initiation and growth perpendicular to the load-
 538 ing direction is observed in the third pattern as well,
 539 which corresponds to the zig-zag (30°) configuration.
 540 Therefore, the crack orientations between 0° to 10.9°
 541 are mainly influenced by the arm-chair pattern. On
 542 the other hand, crack orientations between 22.5° to
 543 30° are mainly influenced by the zig-zag pattern. The
 544 other orientations are influenced by the pattern num-
 545 ber 3. Results demonstrate that the pattern number 1 is
 546 the weakest and the pattern number 2 is the strongest.
 547 Based on the results, $\approx 10\%$ improvement as compared
 548 to an initial arm-chair configuration in yield stress as
 549 well as yield strain could be achieved by selecting the
 550 lattice orientation in relation to the initial notch direc-
 551 tion.

552 3.3 Crack size dependent mechanical properties

553 The variation of stress with strain for arm-chair
 554 Graphene at different percentage of crack length with
 555 respect to the width of the sample is analyzed at 0 K,
 556 see Fig. 10a. The crack size is varied from $a_0 = 0.025L$
 557 to $0.90L$ with total 13 different initial simulated crack
 558 lengths. With the increase in crack size, the amount
 559 of energy required to break the bond around the crack
 560 tip decreases. Hence, the yield stress is also observed
 561 to be decreasing, as shown in Fig. 10a. It is observed
 562 that until $a_0 = 0.10L$ of the crack size, the stiff-
 563 ness remains almost the same. The trend observed in
 564 Fig. 10a is observed to be similar to the variation of
 565 stress with strain for different hole sizes in Zhang et al.
 566 (2012a). However, further increase in crack size leads
 567 to decrease in yield stress as well as the stiffness. On
 568 the other hand, the yield strain is noticed to decrease
 569 initially with an increase in crack size. Whereas, after
 570 a critical crack size, $a_0 \approx 0.20L$, the variation in the
 571 yield strain remains almost constant at 0.05. Also sim-

ilar variations are observed for the zig-zag Graphene at
 ≈ 0 K, as shown in Fig. 10c.

572 In order to understand the effect of temperature on
 573 the mechanical properties of Graphene, preliminary
 574 simulations are performed at room temperature 300 K,
 575 for arm-chair and zig-zag orientations with varying
 576 crack length, as shown in Fig. 10b, d, respectively. It is
 577 observed that even at 300 K, the yield strain becomes
 578 constant after a critical crack length. The variation of
 579 the fracture toughness with a_0/L ratio for arm-chair
 580 and zig-zag orientations at ≈ 0 and 300 K are plotted
 581 in Fig. 10e. From these results, both the arm-chair as
 582 well as the zig-zag orientations show almost constant
 583 fracture toughness values at different temperatures. In
 584 general, $a_0/L < 0.5$ can be considered to predict the
 585 stress-intensity factor. From Fig. 10e, the median val-
 586 ues of mode I fracture toughness of arm-chair/zig-zag
 587 Graphene is found to be $8.4 \text{ MPa}\sqrt{m}$ at ≈ 0 K. The vari-
 588 ation in standard deviation is found to be 1.27. On the
 589 other hand, at 300 K, the median values of mode I frac-
 590 ture toughness of arm-chair/zig-zag Graphene is found
 591 to be $7.4 \text{ MPa}\sqrt{m}$. The variation in standard deviation
 592 is found to be 1.52. A further detailed study on the stress
 593 intensity factor of single layer Graphene at different
 594 temperatures is beyond the scope of present work and
 595 is left for future investigation.

596 Furthermore, to study the combined effect of dif-
 597 ferent orientations and crack sizes on the yield stress
 598 and yield strain, 10 different lattice orientations with
 599 13 different crack sizes are simulated. The distribution
 600 of yield stress and yield strain, with crack length is
 601 plotted in Fig. 11a, b, respectively. Figure 11c shows
 602 the stress-strain distribution with lattice lattice orienta-
 603 tion in a three dimensional plot, for all the initial crack
 604 lengths considered in this paper. Based on Fig. 10a,
 605 for a given orientation, the yield stress decreases with
 606 an increase in crack length, as discussed in Sect. 3.2.
 607 Note that the discussion in Sect. 3.2 is valid for crack
 608 sizes of $a_0 \geq 0.20L$. Smaller crack sizes shows differ-
 609 ent variation in yield stress with varying crack orienta-
 610 tions due to the involvement of the free surface near the
 611 crack tip. The yield strain also shows a decreasing trend
 612 with increase in crack size for a given orientation up to
 613 $a_0 = 0.33L$ of crack length. A constant yield strain of
 614 ≈ 0.05 is observed with further increase in crack size
 615 up to $a_0 = 0.90L$. We report that this is one of the rea-
 616 sons for the softening of the Graphene, as displayed
 617 by the decrease of stiffness with increase in crack
 618 length.

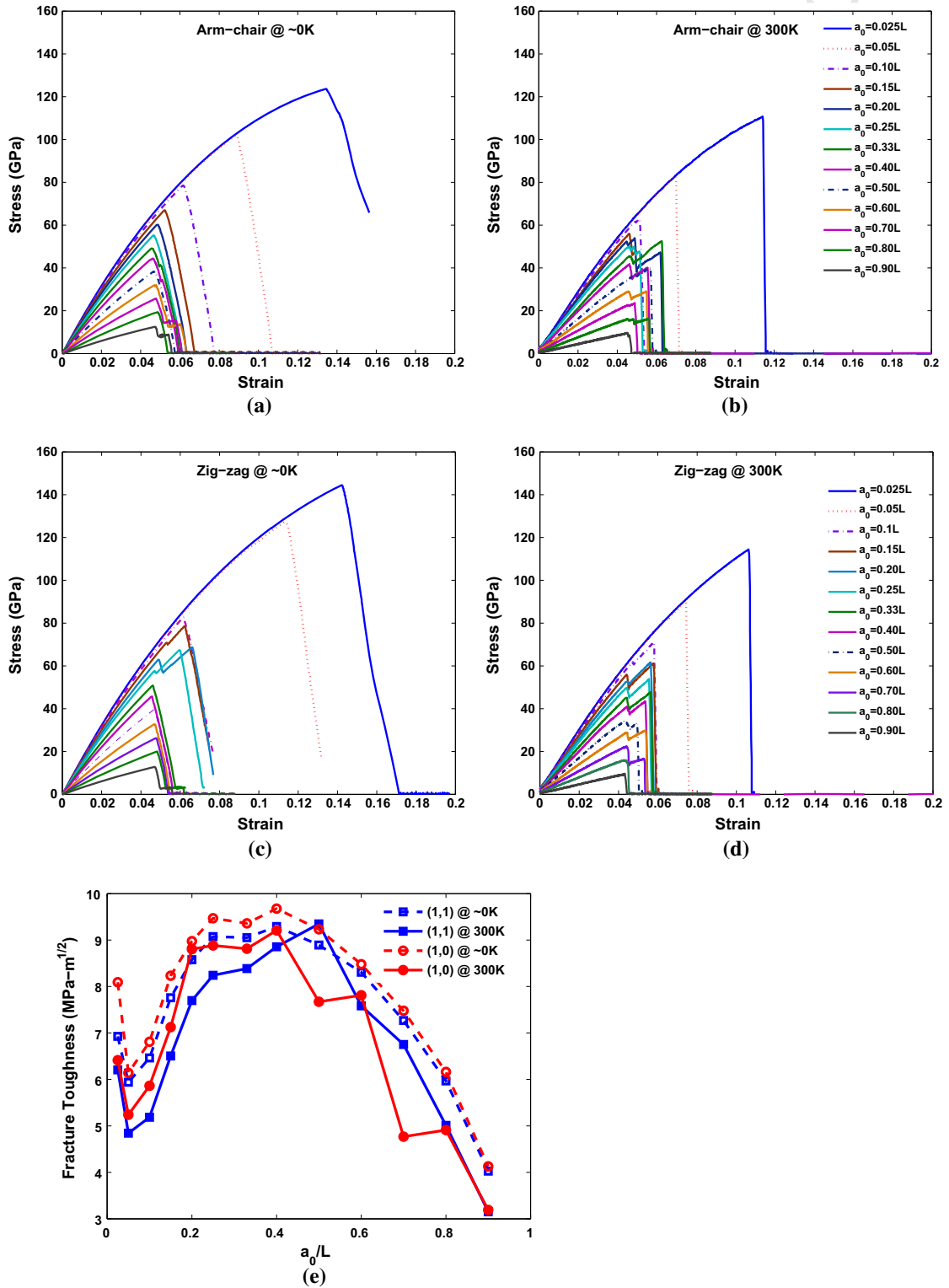


Fig. 10 Stress–strain plots for **a, b** arm-chair and **c, d** zig-zag Graphene at ≈ 0 and 300 K, respectively, for different crack lengths. **e** Variation of fracture toughness in arm-chair and zig-zag Graphene at ≈ 0 and 300 K

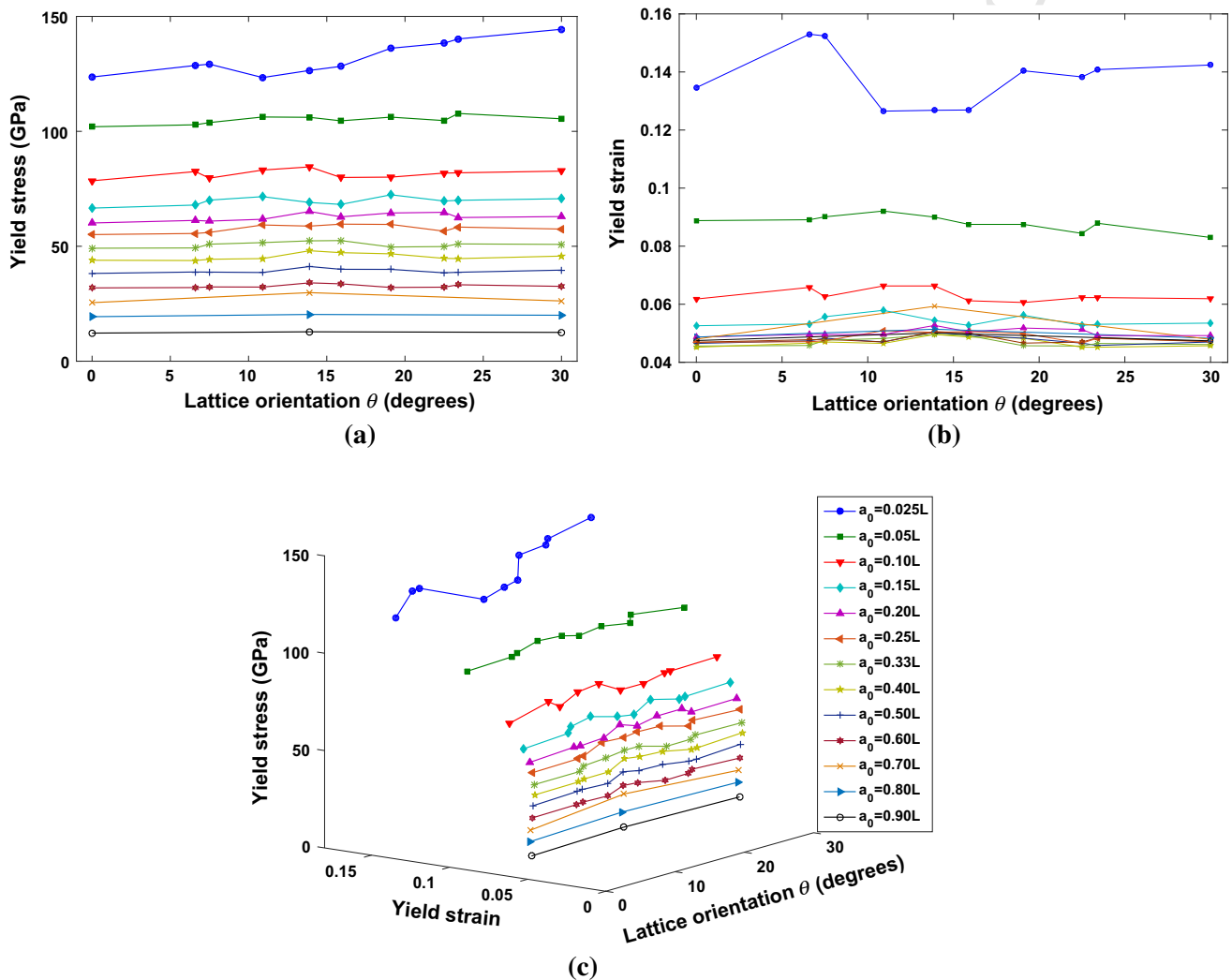


Fig. 11 Variation of the **a** stress and **b** strain, with the lattice orientation, for various crack sizes. **c** Plots **a** and **b** are combined to generate the three dimensional plot, where the variation of

the yield stress and yield strain with the crack orientation can be simultaneously monitored. The legends of plots **a** and **b** are shown in (c)

621 Furthermore, based on the yield stress and yield
 622 strain plotted in Fig. 11a, b, a sudden decrease in
 623 yield stress and yield strain can be noticed for crack
 624 sizes < 10 nm. However, for larger crack sizes a lin-
 625 ear decrease in yield stress is observed, whereas yield
 626 strain remains constant. The behaviour is found to be
 627 the same in all the lattice orientations considered in the
 628 present study. Therefore, the behaviour of yield stress
 629 as well as yield strain with crack length is insensitive to
 630 the orientation, as shown in Fig. 12a, b. The variation
 631 of the yield stress with yield strain for all the orienta-
 632 tions considered in the present work is plotted Fig. 12c.
 633 Based on the results, a yield strain of ≈ 0.05 can be con-
 634 sidered as a critical strain value below which Graphene

635 does not show failure. This information can be utilized
 636 in the design of nano-devices for various strain sensor
 637 applications.

4 Conclusions

638
 639 Tensile deformation of two dimensional Graphene
 640 structure with an edge crack has been simulated based
 641 on molecular dynamics. Application of the load leads
 642 to the bond deformation, resulting in an increase of
 643 the system potential energy and hence the stress along
 644 the loading direction. The severely stressed bonds
 645 are breaking when the stress reaches a critical value,

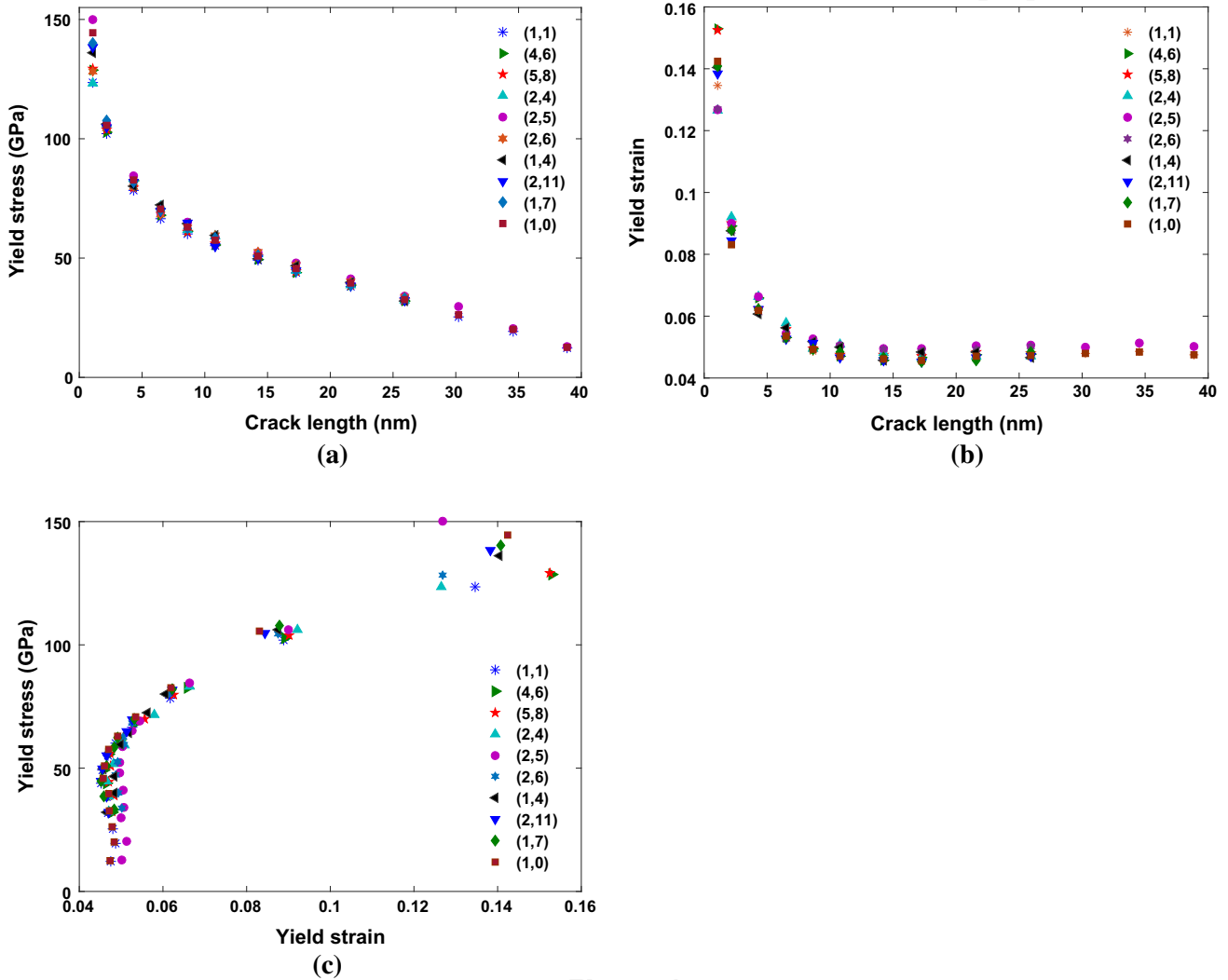


Fig. 12 Atomic configurations near the crack tip for Graphene orientations 0°, 13.9° and 30°

646 exposing the new set of atoms to resist the applied
647 load.

648 Ten different lattice orientations with thirteen dif-
649 ferent initial crack lengths have been considered to
650 study their effect on the yield stress and yield strain
651 of Graphene. Graphene is observed fracture in three
652 particular patterns in all the lattice orientations, where
653 the arm-chair fracture pattern is observed to possess
654 the lowest yield properties. A sudden decrease in yield
655 stress and yield strain is noticed for crack sizes <10 nm.
656 However, for larger crack sizes a linear decrease in
657 yield stress is noticed, whereas a constant yield strain of
658 ≈0.05 is observed. Therefore, the yield strain of ≈0.05
659 can be considered as a critical strain value below which
660 Graphene does not show failure. This information can
661 be utilized in the design of nano-devices for various

662 strain sensor applications. Mode I fracture toughness
663 of arm-chair and zig-zag Graphene is estimated as
664 $8.4 \pm 1.27 \text{ MPa}\sqrt{m}$ and $7.4 \pm 1.52 \text{ MPa}\sqrt{m}$ at ≈0
665 and 300 K, respectively. Furthermore, Graphene can be
666 coated on the Silicon surface to enhance the mechanical
667 (Berardone et al. 2014; Schröder et al. 2012) and
668 electrical characteristics the solar cells (Köntges et al.
669 2011; Paggi et al. 2011, 2013, 2014). The present study
670 will be useful in selecting the optimum orientation of
671 Graphene.

672 **Acknowledgments** B. Javvaji, D. R. Mahaptra and T. Rabczuk
673 gratefully acknowledge the financial support from the Germany
674 Science Foundation (DFG) and from the International Research
675 Staff Exchange Scheme (IRSES), FP7-PEOPLE-2010-IRSES,
676 through the project ‘MultiFrac’. M. Paggi and P. R. Budarapu
677 acknowledges the funding from the European Research Coun-

678 cil (ERC), Grant No. 306622 through the ERC Starting Grant
 679 “Multi-field and multi-scale Computational Approach to Design
 680 and Durability of PhotoVoltaic Modules”—CA2PVM. B. Javvaji
 681 and D. R. Mahapatra thankfully acknowledge the use of com-
 682 putational facilities at the ACECOST Computational Science
 683 Lab, Department of Aerospace Engineering, IISc and funding
 684 under ACECOST Phase-III program of Aeronautics Research
 685 and Development Board, India. Zi appreciates the financial sup-
 686 port through Grant No. 20133010021770, from the New &
 687 Renewable Energy Core Technology Program of the Korea Insti-
 688 tute of Energy Technology Evaluation and Planning (KETEP),
 689 Ministry of Trade, Industry & Energy, Republic of Korea.

690 Appendix: Tersoff potential function

691 The mathematical expression of the bond energy based
 692 on the Tersoff potential is given in Eq. (1). The bond
 693 energy in the Tersoff framework is a combination
 694 of repulsive (f_R) energy function which is exponen-
 695 tially decaying and attractive (f_A) energy function that
 696 exponentially increases; with the increase of distance
 697 between the atoms. f_c is a smooth spherical cutoff func-
 698 tion around atom α based upon the distance to the first
 699 nearest-neighbor shell. The function f_c in Eq. (1) is
 700 defined as Tersoff (1989):

$$701 f_c(r_{\alpha\beta}) = \begin{cases} 1 & \text{when } r_{\alpha\beta} < \mathcal{R}_{\alpha\beta} \\ \frac{1}{2} + \frac{1}{2} \cos\left(\frac{\pi(r_{\alpha\beta} - \mathcal{R}_{\alpha\beta})}{(\mathcal{S}_{\alpha\beta} - \mathcal{R}_{\alpha\beta})}\right) & \text{when } \mathcal{R}_{\alpha\beta} < r_{\alpha\beta} < \mathcal{S}_{\alpha\beta} \\ 0 & \text{when } r_{\alpha\beta} > \mathcal{S}_{\alpha\beta} \end{cases} \quad (3)$$

704 from Eq. (3), f_c returns a value of 1 if $r_{\alpha\beta}$ is less than
 705 $\mathcal{R}_{\alpha\beta}$ and 0 when $r_{\alpha\beta}$ greater than $\mathcal{S}_{\alpha\beta}$. The values of the
 706 constants $\mathcal{R}_{\alpha\beta} = \sqrt{\mathcal{R}_\alpha \mathcal{R}_\beta}$ and $\mathcal{S}_{\alpha\beta} = \sqrt{\mathcal{S}_\alpha \mathcal{S}_\beta}$, (where
 707 α and β can be two different atom types, like Silicon
 708 and Carbon) are listed for Silicon and Carbon atoms in
 709 Tersoff (1989). The repulsive and attractive potential
 710 energies are tuned with the parameters $\mathcal{A}_{\alpha\beta}$ and $\mathcal{B}_{\alpha\beta}$,
 711 respectively. The repulsive potential energy is defined
 712 as Tersoff (1989)

$$713 f_R(r_{\alpha\beta}) = \mathcal{A}_{\alpha\beta} e^{-\mathcal{D}_{\alpha\beta} r_{\alpha\beta}} \quad (4)$$

714 and the attractive potential energy is estimated from
 715 Tersoff (1989)

$$716 f_A(r_{\alpha\beta}) = -\mathcal{B}_{\alpha\beta} e^{-\mathcal{E}_{\alpha\beta} r_{\alpha\beta}} \quad (5)$$

717 where $\mathcal{A} = \sqrt{\mathcal{A}_\alpha \mathcal{A}_\beta}$, $\mathcal{B} = \sqrt{\mathcal{B}_\alpha \mathcal{B}_\beta}$, $\mathcal{D}_{\alpha\beta} = (\mathcal{D}_\alpha +$
 718 $\mathcal{D}_\beta)/2$ and $\mathcal{E}_{\alpha\beta} = (\mathcal{E}_\alpha + \mathcal{E}_\beta)/2$, in Eqs. (4) and (5)
 719 are constants. The variable $b_{\alpha\beta}$ in Eq. (1) is designed

to represent the bond strength of the potential. $b_{\alpha\beta}$ is
 inversely proportional to the coordination number and
 is defined as Tersoff (1989)

$$b_{\alpha\beta} = \xi_{\alpha\beta} \left(1 + \mathcal{P}_\alpha^{q_\alpha} \zeta_{\alpha\beta}^{q_\alpha}\right)^{-1/2q_\alpha} \quad (6)$$

where \mathcal{P} and q are the constants. $\zeta_{\alpha\beta}$ provides a
 weighted measure of the number of other bonds (γ)
 competing with the bond α - β , which is defined as Ter-
 soff (1989)

$$\zeta_{\alpha\beta} = \sum_{\gamma \neq \alpha, \beta} f_c(r_{\alpha\gamma}) g(\theta_{\alpha\beta\gamma}) \quad (7)$$

where $\xi_{\alpha\beta}$ is the strengthening or weakening factor of
 the hetero-polar bonds and $g(\theta_{\alpha\beta\gamma})$ provides a mea-
 sure of dependence on the bonding angle $\theta_{\alpha\beta\gamma}$, sub-
 tended at atom α by atoms β and γ . The variable
 $g(\theta_{\alpha\beta\gamma})$ is included to stabilize the atomic geome-
 try under shear operations and to provide an effective
 coordination contribution based on the elastic energy
 of the current configuration, which is defined as Tersoff
 (1989)

$$g(\theta_{\alpha\beta\gamma}) = 1 + \frac{c_\alpha^2}{d_\alpha^2} - \frac{c_\alpha^2}{d_\alpha^2 + (h_\alpha - \cos(\theta_{\alpha\beta\gamma}))^2} \quad (8)$$

where c_α , d_α and h_α are the constants.

References

- 741 Ansari R, Ajori S, Motevalli B (2012) Mechanical properties
 742 of defective single-layered graphene sheets via molecu-
 743 lar dynamics simulation. *Superlattices Microstruct* 51:274–
 744 289
 745 Berardone I, Corrado M, Paggi M (2014) A generalized electric
 746 model for mono and polycrystalline silicon in the presence
 747 of cracks and random defects. *Energy Procedia* 55:22–29
 748 Bu H, Chen Y, Zou M, Yi H, Bi K, Ni Z (2009) Atomistic simu-
 749 lations of mechanical properties of graphene nanoribbons.
 750 *Phys Lett A* 373:3359–3362
 751 Budarapu P, Javvaji B, Sutrarak V, Mahapatra D, Zi G, Rabczuk
 752 T (2015) Crack propagation in graphene. *J Appl Phys*
 753 118:382–395
 754 Budarapu P, Rammohan B, Vijay S, Satish B, Raghunathan R
 755 (2009) Aero-elastic analysis of stiffened composite wing
 756 structure. *J Vib Eng Technol* 8(3):255–264
 757 Budarapu P, Sudhir S, Brahmanandam J, Mahapatra D (2014c)
 758 Vibration analysis of multi-walled carbon nanotubes
 759 embedded in elastic medium. *Front Struct Civil Eng*
 760 8(2):151–159
 761 Cao G (2014) Atomistic studies of mechanical properties of
 762 graphene. *Polymers* 6:2404–2432
 763 Changgu L, Xiaoding W, Jeffrey WK, James H (2008) Mea-
 764 surement of the elastic properties and intrinsic strength of
 765 monolayer graphene. *Science* 321(5887):385–388

- 766 Chen K, Bin S, Yonghai Y, Juanjuan Q, Lin G (2015a) Binary syn- 825
767 ergy strengthening and toughening of bio-inspired nacre- 826
768 like graphene oxide/sodium alginate composite paper. ACS 827
769 Nano 9(8):8165–8175 828
- 770 Chen M, Quek S, Sha Z, Chiu C, Pei Q, Zhang Y (2015b) Effects 829
771 of grain size, temperature and strain rate on the mechanical 830
772 properties of polycrystalline graphene -a molecular dynam- 831
773 ics study. Carbon 85:135–146 832
- 774 Chuvilin A, Meyer J, Algara-Siller G, Kaiser U (2009) From 833
775 graphene constrictions to single carbon chains. New J Phys 834
776 11:083019 835
- 777 Datta D, Nadimpalli S, Yinfeng L, Shenoy V (2015) Effect of 836
778 crack length and orientation on the mixed-mode fracture 837
779 behavior of graphene. Extreme Mech Lett 5:10–17 838
- 780 Fengnian X, Han W, Di X, Madan D, Ashwin R (2014) Two- 839
781 dimensional material nanophotonics. Nat Photonics 8:899– 840
782 907 841
- 783 Fiori G, Bonaccorso F, Iannaccone G, Palacios T, Neumaier 842
784 D, Seabaugh A, Banerjee S, Colombo L (2014) Electron- 843
785 ics based on two-dimensional materials. Nat Nanotechnol 844
786 9:768–779 845
- 787 Gamboa A, Vignoles G, Leyssale J-M (2015) On the prediction 846
788 of graphene's elastic properties with reactive empirical bond 847
789 order potentials. Carbon 89:176–187 848
- 790 Geim A (2009) Graphene: status and prospects. Science 849
791 324:1530–1534 850
- 792 Grantab R, Shenoy V, Ruoff R (2010) Anomalous strength char- 851
793 acteristics of tilt grain boundaries in graphene. Science 852
794 330:946–948 853
- 795 Hadden C, Klimek-McDonald D, Pineda E, King J, Reichanader 854
796 A, Miskioglu I, Gowtham S, Odegard G (2015) Mechani- 855
797 cal properties of graphene nanoplatelet/carbon fiber/epoxy 856
798 hybrid composites: Multiscale modeling and experiments. 857
799 Carbon 95:100–112 858
- 800 Huhu C, Chuangang H, Yang Z, Liangti Q (2014) Graphene fiber: 859
801 a new material platform for unique applications. NPG Asia 860
802 Mater 6:e113 861
- 803 Jhon Y, Jhom Y, Yoem G, Jhon M (2014) Orientation dependence 862
804 of the fracture behavior of graphene. Carbon 66:619–628 863
- 805 Jhon Y, Zhu S, Ahn J, Jhon M (2012) The mechanical responses 864
806 of tilted and non-tilted grain boundaries in graphene. Carbon 865
807 50:3708–3716 866
- 808 Jin C, Lan H, Peng L, Suenaga K, Iijima S (2009) Deriving carbon 867
809 atomic chains from graphene. Phys Rev Lett 102:205501 868
- 810 Khare R, Mielke S, Paci J, Zhang S, Ballarini R, Schatz 869
811 G, Belytschko T (2007) Coupled quantum mechanical/mole- 870
812 cular mechanical modeling of the fracture of defect- 871
813 ive carbon nanotubes and graphene sheets. Phys Rev B 872
814 75:075412 873
- 815 Kim K, Artyukhov V, Regan W, Liu Y, Crommie M, Yakobson 874
816 B, Zettl A (2012) Ripping graphene: preferred directions. 875
817 Nano Lett 12:293–297 876
- 818 Kim Y, Lee J, Yeom M, Shin J, Kim H, Cui Y, Kysar J, Hone 877
819 J, Jung Y, Jeon S, Han S (2013) Strengthening effect of 878
820 single-atomic-layer graphene in metal-graphene nanolay- 879
821 ered composites. Nat Commun 4:2114 880
- 822 Kinam K, Jae-Young C, Taek K, Seong-Ho C, Hyun-Jong C 881
823 (2011) A role for graphene in silicon-based semiconductor 882
824 devices. Nature 479:338–344 883
- Köntges M, Kunze I, Kajari-Schröder S, Breitenmoser X, Bjrnke- 825
lett B (2011) The risk of power loss in crystalline silicon 826
based photovoltaic modules due to microcracks. Sol Energy 827
Mater Sol Cells 95:1131–1137 828
- Kostarelos K, Novoselov K (2014) Graphene devices for life. Nat 829
Nanotechnol 9:744–745 830
- Kravets V, Jalil R, Kim Y-J, Ansell D, Aznakayeva D, Thack- 831
ray B, Britnell L, Belle B, Withers F, Radko I, Han Z, 832
Bozhevolnyi S, Novoselov K, Geim A, Grigorenko A (2014) 833
Graphene-protected copper and silver plasmonics. Sci Rep 834
4:5517 835
- Liu F, Ming P, Li J (2007) Ab initio calculation of ideal strength 836
and phonon instability of graphene under tension. Phys Rev 837
B 76:064120 838
- Liu J (2014) Charging graphene for energy. Nat Nanotechnol 839
9:739–741 840
- Marc G, McMillan W (1985) The virial theorem. Adv Chem 841
Phys 58:209 842
- Mics Z, Tielrooij K-J, Parvez K, Jensen S, Ivanov I, Feng X, 843
M*ullen K, Bonn M, Turchinovich D (2015) Thermody- 844
namic picture of ultrafast charge transport in graphene. Nat 845
Commun 6:7655 846
- Morpurgo A (2015) Ten years of nature physics: the abc of 2D 847
materials. Nat Phys 11:625–626 848
- Paggi M, Berardone I, Infuso A, Corrado M (2014) Fatigue degra- 849
dation and electric recovery in silicon solar cells embedded 850
in photovoltaic modules. Sci Rep 4:4506 851
- Paggi M, Corrado M, Rodriguez MA (2013) A multi-physics 852
and multi-scale numerical approach to microcracking 853
and power-loss in photovoltaic modules. Compos Struct 854
95:630–638 855
- Paggi M, Kajari-Schröder S, Eitner U (2011) Thermo- 856
mechanical deformations in photovoltaic laminates. J Strain 857
Anal Eng Des 46(8):772–782 858
- Pei Q, Zhang Y, Shenoy V (2010) A molecular dynamics study 859
of the mechanical properties of hydrogen functionalized 860
graphene. Carbon 48:898–904 861
- Peng Z, Lulu M, Feifei F, Zhi Z, Cheng P, Phillip EL, Zheng L, 862
Yongji G, Jiangnan Z, Xingxiang Z, Pulickel MA, Ting Z, 863
Jun L (2014) Fracture toughness of graphene. Nat Commun 864
5:3782 865
- Plimpton S (1995) Fast parallel algorithms for short-range mole- 866
cular dynamics. J Comput Phys 117:1–19 867
- Pospischil A, Furchi M, Mueller T (2014) Solar-energy conver- 868
sion and light emission in an atomic monolayer p–n diode. 869
Nat Nanotechnol 9:257–261 870
- Quan L, Zhen T, Xueqian Z, Ranjan S, Liangliang D, Jianqiang G, 871
Jiaguang H, Weili Z (2015) Active graphene-silicon hybrid 872
diode for terahertz waves. Nat Commun 6:7082 873
- Rodrigues G, Zelenovskiy P, Romanyuk K, Luchkin S, Kopelev- 874
vich Y, Kholkin A (2015) Strong piezoelectricity in single- 875
layer graphene deposited on SiO_2 grating substrates. Nat 876
Commun 6:7572 877
- Santanu S, Elena B, Haddon RC (2012) Covalent chemistry in 878
graphene electronics. Mater Today 15(6):276–285 879
- Sarma D, Adam S, Hwang E, Rossi E (2011) Electronic transport 880
in two dimensional graphene. Rev Mod Phys 83:407–470 881
- Schröder SK, Kunze I, Köntges M (2012) Criticality of cracks 882
in PV modules. Energy Procedia 27:658–663 883

- 884 Schwierz F (2010) Graphene transistors. *Nat Nanotechnol* 5:487–496 930
- 885 5:487–496 931
- 886 Shenderova O, Brenner D, Omeltchenko A, Su X, Yang L (2000) 932
- 887 Atomistic modeling of the fracture of polycrystalline dia- 933
- 888 mond. *Phys Rev B* 61(6):3877–3888 934
- 889 Shin S, Choi H, Shin J, Bae D (2015) Strengthening behavior 935
- 890 of few-layered graphene/ aluminum composites. *Carbon* 936
- 891 82:143–151 937
- 892 Son I, Park J, Kwon S, Park S, Rummeli M, Bachmatiuk A, 938
- 893 Song H, Ku J, Choi J, Choi J, Doo S-G, Chang H (2015) Sili- 939
- 894 con carbide-free graphene growth on silicon for lithium-ion 940
- 895 battery with high volumetric energy density. *Nat Commun* 941
- 896 6:7393 942
- 897 Subramanian A, Sun C (2008) Continuum interpretation of 943
- 898 virial stress in molecular simulations. *Int J Solids Struct* 944
- 899 45:4340–4346 945
- 900 Sun X-Y, Hu H, Cao C, Xua Y-J (2015) Anisotropic vacancy- 946
- 901 defect-induced fracture strength loss of graphene. *RSC Adv* 947
- 902 5:13623–13627 948
- 903 Swope W, Anderson H, Berens P, Wilson K (1982) A computer 949
- 904 simulation method for the calculation of equilibrium con- 950
- 905 stants for the formation of physical clusters of molecules: 951
- 906 application to small water clusters. *J Chem Phys* 76:637 952
- 907 Tersoff J (1989) Modeling solid-state chemistry: interatomic 953
- 908 potentials for multicomponent systems. *Phys Rev B* 954
- 909 39(8):5566–5568 955
- 910 Thomas S, Ajith K (2014) Molecular dynamics simulation of 956
- 911 the thermo-mechanical properties of monolayer graphene 957
- 912 sheet. *Proc Mater Sci* 5:489–498 958
- 913 Tiwary C, Javvaji B, Kumar C, Mahapatra D, Ozden S, Ajayan 959
- 914 P, Chattopadhyay K (2015a) Chemical-free graphene by 960
- 915 unzipping carbon nanotubes using cryo-milling. *Carbon* 961
- 916 217–224 962
- 917 Tiwary C, Vishnu D, Kole A, Brahmanandam J, Mahapatra D, 963
- 918 Kumbhakar P, Chattopadhyay K (2015b) Stabilization of the 964
- 919 high-temperature and high-pressure cubic phase of ZnO by 965
- 920 temperature-controlled milling. *J Mater Sci*. doi:10.1007/ 966
- 921 s10853-015-9394-1 967
- 922 Traversi F, Raillon C, Benameur S, Liu K, Khlybov S, Tosun M, 968
- 923 Krasnozhan D, Kis A, Radenovic A (2014) Detecting the 969
- 924 translocation of DNA through a nanopore using graphene 970
- 925 nanoribbons. *Nature Nanotechnol* 8:939–945 971
- 926 Vadukumpully S, Paul J, Mahanta N, Valiyaveetil S (2011) Flex- 972
- 927 ible conductive graphene/poly(vinyl chloride) composite 973
- 928 thin films with high mechanical strength and thermal sta- 974
- 929 bility. *Carbon* 49:198–205 975
- Volokh KY (2012) On the strength of graphene. *J Appl Mech* 930
- 79(6):064501–064501. doi:10.1115/1.4005582 931
- Weiwei Z, Yanlei W, Zhangting W, Wenhui W, Kedong B, Zheng 932
- L, Juekuan Y, Yunfei C, Zhiping X, Zhenhua N (2015) 933
- Defect-engineered heat transport in graphene: a route to 934
- high efficient thermal rectification. *Sci Rep* 5:11962 935
- Wen S, Yuqi Y, Jiangnan S, Hua C (2012) A graphene-based com- 936
- posite material noncovalently functionalized with a chemi- 937
- luminescence reagent: synthesis and intrinsic chemilumi- 938
- nescence activity. *Chem Commun* 48:2894–2896 939
- Xue T, Peng B, Xue M, Zhong X, Chiu C-Y, Yang S, Qu Y, 940
- Ruan L, Jiang S, Dubin S, Kaner R, Zink J, Meyerhoff M, 941
- Duan X, Huang Y (2014) Integration of molecular and enzy- 942
- matic catalysts on graphene for biomimetic generation of 943
- antithrombotic species. *Nat Commun* 5:3200 944
- Xuechao Y, Youde S, Tao L, Tao(Tom) W, Wang QJ (2015) Pho- 945
- to-current generation in lateral graphene p–n junction created 946
- by electron-beam irradiation. *Sci Rep* 5:12014 947
- Ying-Yan Z, Qing-Xiang P, Yiu-Wing M, Yuan-Tong G (2014) 948
- Temperature and strain-rate dependent fracture strength of 949
- graphynes. *J Phys D Appl Phys* 47(42):425301 950
- Zan L, Genlian F, Qiang G, Zhiqiang L, Yishi S, Di Z (2015) Syn- 951
- ergistic strengthening effect of graphene-carbon nanotube 952
- hybrid structure in aluminum matrix composites. *Carbon* 953
- 95:419–427 954
- Zhang H, Wu J, He J, Zhang Z (2012a) Effect of hole size on the 955
- fracture of graphene nanomesh. In: *Proceeding of the 19th* 956
- European conference on fracture*, ISBN 978-5-905576-18-8 957
- Zhang T, Li X, Kadkhodaei S, Gao H (2012b) Flaw insensitive 958
- fracture in nanocrystalline graphene. *Nano Lett* 12:4605– 959
- 4610 960
- Zhang Y, Zhao J, Wie N, Jiang J, Rabczuk T (2013) Effects of 961
- the dispersion of polymer wrapped two neighbouring single 962
- walled carbon nanotubes (SWNTs) on nanoengineering 963
- load transfer. *Compos Part B Eng* 45(1):1714–1721 964
- Zhao H, Aluru N (2010) Temperature and strain-rate dependent 965
- fracture strength of graphene. *J Appl Phys* 108:064321 966
- Zhao H, Min K, Aluru N (2009) Size and chirality dependent 967
- elastic properties of graphene nanoribbons under uniaxial 968
- tension. *Nano Lett* 9(8):3012–3015 969