Research Article

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Research on the auxetic behavior and mechanical properties of periodically rotating graphene nanostructures

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Abstract: Negative Poisson’s ratio (auxetic) material is one of the most widely studied metamaterials, and recent attempts have been made to discover auxeticity in graphene-based and related carbon-based materials. However, it is shown that negative Poisson’s ratio effect requires special conditions, such as high temperature. Achieving negative Poisson’s ratio effect under large strain at ambient conditions is the key to graphene materials in nano-device applications. In order to discover the auxetic properties of nanostructures under large strain, this article proposes periodically rotating graphene nanostructures (PRGNs) which are the combination of graphene and rotating rigid unit structures. Poisson’s ratio, Young’s modulus, and damage mechanism of PRGNs are investigated using molecular dynamics simulation. It can be possible to conclude that PRGNs can also exhibit auxetic behavior, and their negative Poisson’s ratio effect can be maintained even at large strains ($\varepsilon \approx 0.1$). Poisson’s ratio can be regulated by adjusting the value of the geometry parameters of the graphene sheets (GSs), which comprise the PRGNs, and changed from negative to positive and from positive to negative. Also, the influences of the structural size of GSs and the connection angle between GSs on the mechanical properties are explored, which will provide a theoretical basis for the preparation and performance optimization of GSs and the nano-auxetic properties of materials.

Keywords: graphene, auxetic properties, molecular dynamics, Poisson’s ratio, mechanical properties

1 Introduction

Mechanical metamaterials are artificial structural materials, with extraordinary mechanical properties, composed of period structures, which can create unprecedented effective properties through rational design. Among the numerous mechanical metamaterials available, negative Poisson’s ratio material is one of the most widely studied materials [1–3]. Negative Poisson’s ratio refers to the phenomenon of transverse expansion of a material when it is stretched in the axial direction. This unique mode of tensile expansion and deformation gives negative Poisson’s ratio materials many excellent mechanical properties, such as excellent shear strength, indentation strength, fracture resistance, adjustable permeability, and good energy absorption properties [4], which make them very promising for aerospace [5], automotive [6], biomedical, and textile industry [7] application prospects, and is a research hot-spot in the field of materials science.

Auxetic materials can be classified according to geometry and deformation mechanism such as molecular network structures [8], re-entrant structures [9], chiral or anti-chiral structures [10], rotating rigid unit (RRU) structures [11], fiber/node structures [12], origami structures [13], fold structures [4], and bending-inducing structures [14].

The RRU mechanism is one of the most famous mechanisms for inducing auxetic behavior in the designed structure. Rotating rigid structures include rotating square structure, rotating rectangular structure, rotating parallelogram structure, rotating triangle structure, and so on. These models consist of rigid polygons arranged periodically, and the polygons are connected by hinges at the nodes. When the structure is stretched horizontally, these rigid polygons rotate, causing the structure to extend laterally and exhibit a negative Poisson’s ratio effect.

The rotating rigid square structure was first proposed by Grima and Evans in 2000 [15], the results show that Poisson’s ratio of the structure is related to the angle
between two adjacent squares, and Poisson’s ratio of the rotating square rigid body structure can reach −1. Later, Grima et al. [16] developed a “rotating semi-rigid squares” model to describe the predicted auxetic behavior in zeolites with a “rotating squares” nanostructure. Then, they extend the research on two-dimensional (2D) rotating rigid quadrilaterals and discuss the shape and size of the rhombi and the temperature affecting the auxeticity [17]. Also, Grima et al. [18] found that Poisson’s ratios were a function of the shape and relative size of different rectangles and the angle between them in different-sized squares and rectangles. Attard and Grima [19] extended the 2D model to a three-dimensional (3D) structure constructed by rigid cuboids, which deform through the relative rotation of the units, and the negative values of Poisson’s ratio also be found. Gatt et al. [20] present a new class of hierarchical auxetics based on the RRU mechanism. Mizzi et al. [21] presented performance systems that offer the opportunity to exhibit giant negative Poisson’s ratios. Slann et al. [22] studied negative Poisson’s ratio effect of rotating rectangles and rhombuses through numerical modeling and experiments. Rotating rhombuses have been successfully implemented in the manufacture of the esophagus using laser cutting and die-casting techniques. Attard et al. [23] studied the negative linear compressibility of RRs, and the results showed that when hydrostatic pressure is applied, some RRs with specific geometric features and connectivities will expand rather than contracting. Dudek et al. [24] studied the deformation mechanism of auxetic hierarchical rotating square systems through a dynamics approach. Attard et al. [25] studied the filtration properties of a class of negative Poisson’s ratio structures that achieve their auxeticity through an RRU mechanism. Farrugia et al. [26] coupled a 2D rotating rigid body element or a chiral structure to a push-drilling mechanism to create a novel 3D negative Poisson’s ratio structure. Gambin et al. [27] studied the mechanical properties of a kind of polymorphs-ice X through density functional theory simulations. Studies showed that ice X has an auxetic behavior at 45° off-axis in the (100), (010), and (001) planes, and predicted negative Poisson’s ratio can be attributed to the interplay between distortion and hinging of the two orthogonally interconnected rhombi.

The relaxed and axially stretched states along the ox-direction of the rotating rigid rectangular structure are shown in Figure 1 [11], where a and b denote the length and the width of the rotating rigid rectangle, respectively, and θ denotes the pinch angle.

It is shown that among the artificially designed negative Poisson’s ratio materials, the RRU is one of the simplest negative Poisson’s ratio structures, whether at the macroscopic, microscopic, or nano-scale, which has the characteristics of structural simplicity, obvious Poisson’s ratio effect, and easy design. However, the current RRU designed based on metallic materials can only be observed with auxeticity behavior at very small strains (ε < 0.02) [28], which restricts the application of this structure under large strain, and it is necessary to design the material and structure to discover negative Poisson’s ratio effect of rotating rigid structure under large strain conditions.

Carbon nanomaterial is one of the most active research fields in nanotechnology, and GS is the representative material that has attracted a wide range of attention. Due to its superior mechanical [29], electrical [30], optical [31], and thermal [32] properties relative to the other materials, GS has spurred many new applications in materials enhancement [33], sensors [34], drug transportation [35], nanoelectronics, and nano-devices [36]. However, recent attempts have been made to discover auxeticity behavior in graphene-based and related carbon-based materials [37–42].
Grima et al. [37] found that graphene can be used to obtain negative Poisson’s ratio effect by introducing vacancy defects. Graphene monolayers engineered to adopt a corrugated conformation also were found to exhibit a very significant negative Poisson’s ratio upon uniaxial stretching in specific directions [43]. Goldstein et al. [44] analyzed the elastic properties of hexagonal crystals under pressure and found seven crystals with a negative Poisson’s ratio. Openov and Podlivaev [45] simulated the elastic properties of phagraphene and found that the nonplanar configuration has a negative Poisson’s ratio. Rysaeva et al. studied the mechanical properties of fullerenes [46], fullerenes (diamond-like phases based on other fullerene-like molecules) [46,47], tubulanes (diamond-like phases based on carbon nanotubes) [48], and graphene-based diamond-like phases [49] and found negative Poisson’s ratio. The research results show that the graphene-based materials with negative Poisson’s ratio effect require special conditions, such as high temperature [50], high pressure [42], and special chemical treatment [51]. How to achieve negative Poisson’s ratio effect under large strain at ambient conditions is the key to graphene materials in nano-device applications.

To realize negative Poisson’s ratio properties of nanostructures under large strain, this article combines graphene and RRU structure to design periodically rotating graphene nanostructures (PRGNs). Poisson’s ratio, Young’s modulus, and damage mechanism of PRGNs are investigated by molecular dynamics (MD) simulation. The influences of the structural size of GSs and the connection angle between GSs on the mechanical properties are explored, especially negative Poisson’s ratio, which will provide a theoretical basis for the regulation of negative Poisson’s ratio.

2 Simulation method

PRGNs are made of several GSs connected as shown in Figure 2. The model is implemented in VMD software by MATLAB programming. As shown in Figure 2, a indicates armchair-shaped edge, and b indicates zigzag-shape edge. The connection between GSs is hexagonal structures with defects containing S–W defects. The overall sheet model is similar to “Rotating Rigid Unit (RRU).”

The Datafile can be exported after establishing the periodic graphene model, and the Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is used to predict the mechanical response of the PRGNs. MD simulation is a reference to a large number of parallel simulators using large-scale atoms/molecules, with adaptive intermolecular reaction empirical bond-order (AIREBO) potential, which has proven to accurately calculate bond interactions, bond breaks, and bond reconstructions of carbon atoms.

To model the periodic structures, periodic boundary conditions are applied in all directions. The Polak–Ribiere version of the conjugate gradient algorithm is used to minimize the energy of the system, and the conjugate gradient method is used [52] for all conjugate gradient minimum optimization methods with a capacity of $10^{-16}$ eV. After the system reaches the equilibrium state of energy minimization, the system is run in the constant-pressure, constant-temperature ensemble under the conditions of room temperature of 300 K and pressure of 0 Pa, relaxing for a relatively long time to reach the equilibrium state.

After relaxing the initial configuration to obtain the minimum energy configuration, the PRGNs are stretched by applying external displacement of the atoms at the top end while keeping the other end fixed to simulate tension. The displacement is applied step by step, and in each step, the system is relaxed for a certain period of time to reach a new equilibrium state and a new configuration in a canonical ensemble, the so-called canonical ensemble, in which the information of each atom, the energy and temperature of the system, etc., can be obtained. The simulation in the present study is carried out at a strain rate of 0.001/ps, which was applied by the displacement of the atoms at the top end of the periodic graphene structure. During the simulation, the Nosé–Hoover thermostat technique is implemented to reach the equilibrium thermodynamic state at a certain constant temperature at 300 K.
The value of Poisson’s ratio is the negative of the ratio of transverse strain to the axial strain. When the material is stretched in only one direction, differential Poisson’s ratio can be used to describe the mechanical properties of the structure under large strain.

In this article, different models were constructed by varying the values of the edge lengths $a/b$ on both sides of the rectangular graphene and the angle between the two GSs, and then, simulations were performed by MD methods to calculate the strains in the $x$- and $y$-directions, and the strains in the linear segment were taken to be between 0 and 0.05, and Poisson’s ratios were obtained by linear fitting. And the axial stretching operation was performed in the $x$- and $y$-directions, respectively. For each model, five simulations were performed, the mean and standard deviation were counted, and error bars were made.

3 Results and discussion

Figure 3 shows the stress–strain curves of $3 \text{ nm} \times 3 \text{ nm}$ single-layer perfect graphene stretched along the armchair direction. As can be observed in Figure 3 at the first stage, the stress increases linearly with the strain increasing due to the elastic deformation of carbon–carbon bonds. With the continuation of the stretching, the deformation is aggravated. Then, in the next stage, the stress–strain curve performs a nonlinear relation due to the non-linear deformation of the C–C bond and the change of the bond angle, and finally, material damages when the ultimate stress is achieved. Young’s modulus of perfect graphene is about 0.967 TPa, and the damage strength is 102 GPa. This is very close to Young’s modulus of perfect graphene predicted by Liu et al. [53] using the first principle which is 1.05 TPa and the breaking strength is 110 GPa, and Young’s modulus of graphene obtained by Lee et al. [54] using the nanoindentation test is 1.02 TPa and the breaking strength is 123.5 GPa. This shows that the perfect graphene tensile stress–strain curve is in general agreement with the reference, thus verifying the feasibility of the simulation method.

According to the above simulation method, MD simulations were used to stretch the relaxed PRGNs in the $x$-direction, and their stress–strain curves were obtained (as shown in Figure 4). It can be observed in Figure 4 that the stretching process is accompanied by the elongation of the C–C bond until it breaks. Graphene also gradually deforms from a regular hexagonal structure and finally becomes irregular until fracture. The fracture is located at the junction between GSs because it is the weak link in the structure, and PRGNs have S–W defects at the junction between GSs, which are prone to fracture. When the axial stretching is just carried out, the structure is in the elastic deformation stage, and the rotation between GSs occurs at this stage, at this time, as the strain increases, the stress also grows linearly, and as the stretching continues, the deformation collects, the C–C bond undergoes inelastic deformation, while the angle between the C–C bonds changes and the linear relationship between stress and strain is broken, and finally, the weak point of the structure (the connection

![Figure 3: Stress–strain curves of single-layer perfect graphene: the size is $3 \text{ nm} \times 3 \text{ nm}$.

![Figure 4: Stress–strain curve of rectangular graphene with rotating period under $x$-direction tensile condition: $a = b = 3 \text{ nm}$, $\theta = 150^\circ$.](image-url)
between GSs) where the C–C bond tension reaches its maximum and breaks, followed by a decrease in stress. The stress–strain curve can reflect the basic mechanical parameters, such as the ultimate strength, ultimate strain, and elastic modulus of the structure, and is a major basis for characterizing the mechanical properties of materials.

From the comparison of Figures 3 and 4, it can be easily found that the breaking strength, fracture strain, and Young’s modulus of PRGNs are far lower than those of the perfect graphene. The fracture strain, Young’s modulus, and fracture strength of PRGNs are about 50, 7, and 5% of those of perfect graphene when \( a = b = 3 \text{ nm} \) and \( \theta = 150^\circ \), respectively. And the stress–strain curve of PRGNs is not smooth enough. This is because PRGNs are joined by GSs, and the joint can be considered as defective graphene, and the C–C bond is constantly breaking and reorganizing during the stretching process, which leads to fluctuations in the stress–strain relationship, unlike the smooth stress–strain curve of perfect graphene. Young’s modulus and fracture strength of PRGNs are also much lower than those of perfect graphene. It is suggested that the joint between the GSs of PRGNs is considered to be a gap in the graphene, and the stress concentration will occur at the tip of the gap, which greatly reduces the fracture strength and Young’s modulus of PRGNs. Furthermore, the ultimate strain of PRGNs is lower than that of perfect graphene, and PRGNs are more prone to fracture than perfect graphene and cannot withstand large strains. However, the breaking strain of PRGNs has been greatly improved compared to that of a metallic material with the same structure. In a study of metallic materials based on the RRU mechanism, researchers only found a negative Poisson’s ratio effect at strains less than 0.02 [28]. While the fracture strain of PRGNs structure is about 0.1, which is five times higher than that of RRU metal structure. After reaching the ultimate strength, the stress–strain curve decays oscillatory. This is because, after the C–C bond of graphene breaks, the atoms recombine to form a chain-like structure. This structure may have a certain stretching capacity. As the stretching proceeds, the strain gradually increases and the chain-like system gradually collapses. However, since the breakage is not simultaneous, i.e., there is time lag, the stress–strain curve oscillates irregularly until complete breakage.

Figure 5(a) and (b) show the configuration of PRGNs in equilibrium before stretching and when the uniaxial load is applied in the \( x \)-direction. As can be seen from Figure 5, the stretching process of PRGNs is accompanied by the deformation of GSs as well as the rotation between GSs, and it is the rotation between GSs that causes the stretching process to produce a larger transverse dimension of the structure, resulting in a negative Poisson’s ratio effect. Figure 6 shows the variation pattern of \( y \)-directional strain with \( x \)-directional strain during the stretching of

![Figure 5](image-url)
According to the calculation formula of Poisson’s ratio, exhibits an increase in size in both the x- and y-directions. According to the calculation formula of Poisson’s ratio \( (\nu = -\varepsilon_y/\varepsilon_x) \), it can be observed that Poisson’s ratio of the PRGNs is negative. Figure 6 also shows that PRGNs exhibit more plastic properties than metal and fracture in large strains.

For comparison with metallic materials, PRGNs can exhibit auxetic behavior in larger strains. In a study on periodic porous metal structures based on the RRU mechanical \([28]\), a negative Poisson’s ratio was observed only in a relatively small range of strains \((\varepsilon < 0.02)\). If the material of the structure changes from graphene to metal, due to their geometrical conditions, stress concentrations tend to occur where the rectangles are connected, which in turn exceed the yield stress of the metal and cause damage. Therefore, the range of metallic structures that exhibit auxetic behavior is limited. In contrast, PRGNs exhibit auxetic behavior over a wide range of strains due to their very high resistance to harm and the nature of their covalent bonds.

According to Grima et al. \([11]\), the magnitude of Poisson’s ratio in a RRU structure is determined by the following equation:

\[
\nu_{21} = (\nu_{12})^{-1} = \frac{a^2 \sin^2 \left(\frac{\theta}{2}\right) - b^2 \cos^2 \left(\frac{\theta}{2}\right)}{a^2 \cos^2 \left(\frac{\theta}{2}\right) - b^2 \sin^2 \left(\frac{\theta}{2}\right)}.
\]

(1)

In particular, when \(a = b\), no matter what value \(\theta\) takes, there are:

\[
\nu_{21} = \nu_{12} = -1.
\]

(2)

where \(\nu_{ij}\) represent Poisson’s ratios in the Oxij plane for loading in the Oxj direction, defined by the following equation:

\[
\nu_{ij} = (\nu_{ji})^{-1} = -\frac{\partial \varepsilon_j}{\partial \varepsilon_i}, \quad i, j = 1, 2.
\]

(3)

Eq. (1) illustrates that the magnitude of Poisson’s ratio of a rotating rigid structure in an ideal state is determined by two factors: the value of the aspect ratio \(a/b\) and the magnitude of the angle \(\theta\) between the rectangular sheets. To investigate the influencing factors of Poisson’s ratio, the variation law of Poisson’s ratio size is studied by adjusting the aspect ratio of graphene \(i.e.,\) the value of \(a/b\). Seven models are constructed, keeping \(b = 3\) nm and \(\theta = 150^\circ\) constant and changing the aspect ratio with the value of \(a\) as a variable, in which \(a\) is taken as 1, 1.5, 2, 3, 4.5, 6, and 9 nm. And the same stretching operation is performed in LAMMPS software to calculate the change in the magnitude of its Poisson’s ratio.

It can be seen from Figure 7 that when the value of \(a/b\) changes, Poisson’s ratio also changes. When the aspect ratio \(a/b\) varies in the range of \(1/3\) to \(3\), the value of Poisson’s ratio undergoes the process of changing from positive to negative and then from negative to positive. It can be seen that the magnitude of Poisson’s ratio depends on the value of aspect ratio \(a/b\). Figure 7 also illustrates that the modulation of Poisson’s ratio value can be achieved by adjusting the value of aspect ratio \(a/b\). It can be seen that even a nanoscale structure can have a negative Poisson’s ratio effect, and the size effect has less influence on the structure.

Comparing the structure simulated by MD with the calculated result of Eq. (1), it is found that there are differences between them. For example, when \(a = b\), the theoretical value of Poisson’s ratio calculated by equation (1) is \(-1\), while the consequence of MD simulation is only \(-0.6\). This is because, in the ideal model \([11]\), it is assumed that the rectangle of the periodic structure simply undergoes free rotation without resistance, thus creating a tendency to expand outward, leading to the negative Poisson’s ratio. In our MD simulation, when the structure is stretched, the rectangle rotates with resistance, and the rectangle itself deforms in shape. The rotation of the rectangle leads outward resulting in a negative Poisson’s ratio effect, but due to the resistance, the rectangle is not so easy to rotate and expand outward, which leads to a smaller negative Poisson’s ratio than the calculated value of the formula. Furthermore, in the simulation of MD, the actual shape deformation of the rectangle.
occurs, making the strain in the stretching direction larger, while according to the definition of Poisson’s ratio, that is, the ratio of transverse contraction to longitudinal stretching strain, the strain in the stretching direction becomes larger, resulting in a smaller Poisson’s ratio, so there is a difference with the results in equation (1).

To explore the influence of the connecting angle of the GSs on the mechanical properties, both sides $a$ and $b$ of the GSs were fixed to 3. The effect of angle on Poisson’s ratio of the PRGNs was explored by adjusting the angle of the connection between the GSs. Five models of 30°, 60°, 90°, 120°, and 150° with a gradient of 30° are conducted, and by stretching the PRGNs axially in the $x$-direction and $y$-direction separately, the obtained Poisson’s ratio varies with the angle as shown in Figure 8.

From Figure 8, it can be seen that only changing the angle between the GSs of PRGNs while keeping the value of $a/b$ constant makes the overall Poisson’s ratio of PRGNs change, and Poisson’s ratio of PRGNs shows a trend of increasing and then decreasing with the increase in the angle between the GSs, and further away from 90°, the smaller the Poisson ratio is, i.e., the negative value is larger, and Poisson’s ratio is maximum at 90°, the more it tends to be 0, which seems to be contrary to the conclusion of equation (2). The reason for this is that negative Poisson’s ratio effect of PRGNs is due to the rotation between GSs caused by axial stretching, which in turn increases the lateral dimension. When the angle between two GSs is far from 90°, the stretching of PRGNs leads to the rotation of the GSs, and the rotation tends to stop when the GSs are perpendicular to each other; that is, the angle between GSs is 90°, at that time the stretching of PRGNs only leads to the increase of axial strain until the structure fractures. Therefore, when the angle is farther away from 90°, the more negative Poisson’s ratio effect can be expressed, the more it can rotate. In contrast, when the angle between GSs is 90°, because the rotation limit has been reached, the structure can hardly rotate anymore and the structure can only fracture with the increase in axial strain, so when the angle between GSs is 90°, negative Poisson’s ratio effect is not reflected because the structure can hardly rotate.

In general, there are differences between the structure of PRGNs and “RRU” in the study by ref. [11]. The main differences are the following:

1) The rectangle and the rectangle in the “RRU” model are connected by a hinge. The hinge is ideal and can rotate freely without resistance. The connecting between the rectangles is defective graphene. There is resistance when connecting, stretching, and rotating, and the resistance will lead to stressing concentration. 

2) The “RRU” is assumed that a rectangle is a rigid unit; that is, the rectangle cannot be deformed. When the structure is stretched, only the rotation between rectangles occurs. In our model, the PRGNs can be deformed during the stretching process. Both the deformation of the rectangular graphene and the rotation between the rectangular graphene will occur.

To further investigate the effect of stress concentration at the GS junction on the performance of PRGNs, the von Mises stress distributions were studied for two models with different $a/b$ ratios, in which $a/b = 1$ and $a/b = 0.5$, to investigate the variation law of equivalent effective stresses during the stretching process, and the obtained results are shown in Figure 9.
As can be seen in Figure 9, when the strain is 0.05, the extreme values of the von Mises stress of the PRGNs are mainly concentrated at the tips of the GS joints. As mentioned before, under the stretching action, the GS not only rotates around the connection but also deforms at the same time. By comparing Figure 9(a) and (b), it can be seen that decreasing the ratio of \(a/b\) under the same strain of action leads to an increase in the equivalent force at the connection; that is, the rectangular GS produces a more pronounced stress concentration phenomenon than the square GS. Interestingly, the equivalent force inside the GS should have been larger under tensile loading, but because the GS can generate rotation around the connection, a portion of the energy is consumed in the rotational deformation, and the equivalent force inside the graphene is relaxed. The energy consumed in the rotation is then reflected in the instantaneous increase in the equivalent force at the tip of the connection, i.e., the stress concentration. As can be seen from Figure 9, the free rotation of the GS is restricted in both models, and the higher the equivalent force means, the higher the rotational restriction, and since it cannot rotate freely, negative Poisson’s ratio effect is not as obvious as that of the RRU structure, which is reflected in the smaller absolute value of negative Poisson’s ratio. As shown in Figure 9, the stress concentration at the tip of the GS junction is larger for the PRGNs with \(b = 6\) nm than that for the PRGNs with \(b = 3\) nm. Therefore, its negative Poisson’s ratio effect is not as obvious as that of the PRGNs with \(b = 3\) nm (as shown in Figure 7). In addition, the stress concentration at the tip of the junction also leads to the fracture of the structure at the junction.

Then, the linear segment of the stress–strain curve is taken for linear fitting to calculate Young’s modulus. Young’s modulus of the above seven models is shown in Figure 10.

![Figure 9: von Mises stress distribution of structure with strain of 0.05: (a) \(b = 3\) nm; (b) \(b = 6\) nm.](image)

![Figure 10: Curve of Young's modulus versus \(a/b\) value (stretched in the x-direction).](image)

It can be seen from Figure 10 that, with all other conditions kept constant, when the value of \(a/b\) is in the range of 1/3–3, Young’s modulus shows a gradual decrease when the value of \(a/b\) is gradually increased, from a maximum of 123 GPa to a minimum of 62 GPa, decreased by 49.59%. And Young’s modulus decreases rapidly when \(a/b\) is between 1/3 and 2/3, from 123 to 79 GPa, decreased by 35.77%, indicating that adjusting the value of \(a/b\) at this stage has a great influence on Young’s modulus of the structure; within the stage of \(a/b\) at 2/3–3, Young’s modulus gradually tends to slow down, the slope of change is not as large as at the stage of 1/3–2/3, and Young’s modulus decreases from 79 to 62 GPa, decreased by 21.52%, indicating that the adjustment of the value of \(a/b\) has little effect on Young’s
modulus of the structure during this stage. Overall Young’s modulus is much lower than that of perfect graphene.

4 Conclusions

In this article, the mechanical properties of PRGNs are investigated by MD methods, and the influence laws of the geometric parameters of the structures on the changes of their Poisson’s ratios, fracture mechanisms, stress–strain curves, ultimate strengths, ultimate strains, and Young’s moduli are studied, and the mechanisms are analyzed. Also, auxetics behavior is emphasized. The following conclusions can be drawn.

1) PRGNs can also exhibit auxetic behavior, and its negative Poisson’s ratio effect can be maintained even at large strains (ε ~ 0.1), and it is much more resistant to strain Poisson’s ratio effect of PRGNs, which is due to the rotation bigger than conventional materials such as metals. The negative between GSs is caused by axial stretching, which in turn increases the lateral dimension. The more the GS can rotate freely around the connection, the stronger its negative Poisson’s ratio effect.

2) Compared with perfect graphene, the ultimate strain and fracture strength of the periodically rotated graphene structure are much smaller and the structure is more susceptible to damage because the PRGNs can be viewed as defective graphene, so it is more susceptible to fracture.

3) Poisson’s ratio can be regulated by adjusting the geometry a/b of the GSs, which comprise the PRGNs; that is, Poisson’s ratio can be changed from negative to positive and from positive to negative.

4) Young’s modulus of the structure can be changed by adjusting the GS geometry value a/b. In the range of 1/3 ≤ a/b ≤ 3, Young’s modulus decreases as the value of a/b increases, wherein the range of 1/3 ≤ a/b ≤ 2/3, the curve is steeper, indicating that in this range, Young’s modulus decreases significantly with the increase of a/b value, at 2/3 ≤ a/b ≤ 3, Young’s modulus decreases as the value of a/b increases, but it is not obvious, and the curve tends to slow down.

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