Simulation Study on Tensile Mechanical Properties of Graphene Based on Long and Short-Term Memory Neural Network

Li Ang[1(✉)] and Wang Hui-jun[2]

[1] Basic Education School, Zhuhai College of Jilin University, Zhuhai 519041, China
liang35789@yeah.net
[2] Xinhua College of Ningxia University, Yinchuan 750021, China

Abstract. The current simulation methods of graphene tensile mechanical properties have not processed the data used in the simulation process, resulting in large errors between the simulation results and the experimental results. For this reason, a graphene tensile mechanics based on long and short-term memory neural networks is proposed. The graphene nanoribbons model was established using Materials Studio software to determine the simulation process of graphene tensile mechanical properties. Use the long and short-term memory neural network to process and store the simulation research data to get the simulation results. Analysis of the simulation results shows that the tensile properties of graphene are affected by the structure of graphene itself, the constituent element atoms, and the distance between atoms, and there will be certain differences in tensile forces in different directions. Three sets of comparative experiments are designed. The experimental results show that the simulation results obtained by the simulation method of graphene tensile mechanical properties in this study are very close to the experimental results, and there is basically no experimental error.

Keyword: Long and short term memory neural network · Graphene · Tensile mechanics · Performance simulation

1 Introduction

Graphene is a two-dimensional periodic honeycomb lattice structure composed of six membered rings of carbon, which is a new low dimensional carbon material [1]. In recent years, due to its unique electrical, thermal, mechanical and magnetic properties, graphene has become one of the hot spots in the field of materials science and condensed matter physics in recent years. The research shows that graphene has extremely excellent mechanical properties and is closely related to the chemical bond and electronic structure between carbon atoms. All of them are composed of the strongest chemical bond α in nature all carbon atoms are bound in the same plane, which makes them have ultra-high strength, stiffness and toughness as well as unique deformation mechanism. Therefore, many scholars have actively studied the mechanical properties of graphene [2, 3]. At

W. Fu et al. (Eds.): ICMTEL 2021, LNICST 387, pp. 51–63, 2021.
https://doi.org/10.1007/978-3-030-82562-1_5

present, domestic and foreign scholars' research on graphene is mainly focused on the preparation, characterization, and physical and chemical properties of graphene. Experimental testing, numerical simulation, and theoretical analysis are mostly used to study the mechanical properties of graphene. The research on its mechanical properties is basically at the initial stage, especially the lack of research on the tensile mechanical properties of graphene, resulting in the tensile properties of graphene, which has not been well applied [4]. At present, there are many researches on using neural network to simulate mechanical properties. However, because long-term and short-term memory neural network improves the long-term dependence problem in RNN, it is usually better than time recurrent neural network and hidden Markov model. Moreover, as a nonlinear model, the network can be used as a complex nonlinear unit to construct a larger deep neural network. Compared with convolution neural network [5] and other methods, it has obvious advantages, so in this study of graphene tensile mechanical properties, long-term and short-term memory neural network is used to minimize the training error and improve the simulation accuracy of graphene tensile mechanical properties.

2 Design of Simulation Method for Tensile Mechanical Properties of Graphene

2.1 Building a Graphene Model

Materials Studio software is used to establish the graphene model. In the materials Studio software, a single-layer square graphene nanobelt model with the size of 122.14 nm * 122.14 nm is established by expanding the unit cell, as shown in Fig. 1.

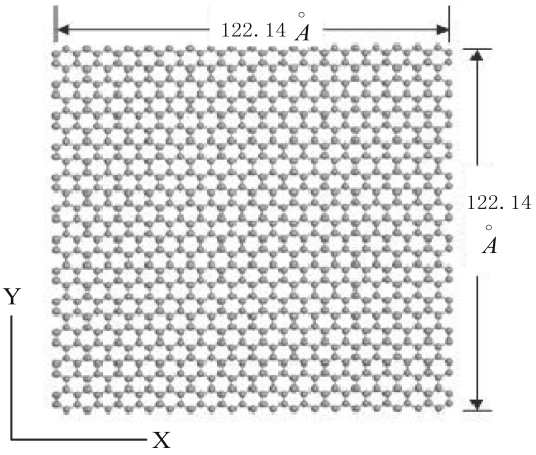


Fig. 1. Graphene model

The graphene nanoribbon model system contains 5800 atoms, the distance between carbon-carbon bonds is 1.42° A, the mass of carbon atoms is 12.0107, and the mass unit is atomic mass unit (1 atomic mass unit = $1.6605402*10^{-27}$ kg), the density of the

polymer is 1.1 g/cm2. According to the study on the tensile mechanical properties of graphene, the required graphene structure is appropriately cut to the edge of the graphene to obtain two different properties of graphene nanoribbons, armchair type and zigzag type, to improve graphene stretching research precision of mechanical properties. Based on the graphene geometric model shown in Fig. 1, the basic geometric properties of the graphene studied in this study can be determined and used as a reference condition for simulating the tensile mechanical properties of graphene.

The graphene model is a honeycomb like two-dimensional crystal composed of single-layer hexagonal cell carbon atoms. The thickness is about 0.335nm, and the length of carbon carbon bond is about 0.142 nm. The final graphene model is square, and the corresponding chiral angles are 0.00°, 5.82°, 10.98°, 15.30°, 19.11°, 24.11°, 25.28°, 27.80° and 30.00° respectively.

2.2 Determine the Simulation Process of Graphene Tensile Mechanical Properties

In the process of studying the tensile mechanical properties of graphene, the graphene model was established and the simulation process of graphene tensile mechanical properties was designed. In the simulation process, the mass of C atom is selected as 12. Control the x direction as a free boundary condition, the y direction as a free boundary condition, and the z direction as a periodic boundary condition. The AIREBO potential function is selected and the long and short-term memory neural network is the default integration algorithm.

Due to the doping of some other elements in graphene materials, it will have a certain impact on the material properties of graphene [6]. However, the radius of silicon atom in graphene is larger than that of carbon atom. The substitution of silicon atom for carbon atom will cause crystal structure distortion, increase the potential energy of graphene, and its stability and mechanical properties will be affected. In order to prevent the whole graphene from being affected too much, the tensile mechanical properties of graphene films with low doping ratio were studied. At this time, the tensile mechanical properties of graphene were simulated as follows:

(1) Simulation of the relaxation characteristics of graphene. Without imposing any external load constraints on the model, the Nose-Hoover thermal bath method is used for temperature adjustment, the control temperature is 0K, the time step is 1fs (Note, $1fs = 10^{-3}ps$), and the entire model is fully unconstrained relaxation.
(2) Tensile simulation of graphene in x direction. The temperature was regulated by Nose-Hoover heat bath method. The temperature was controlled at 0k and the time step was 1FS. The carbon atoms at the left end of the film were fully relaxed, and then the right carbon atoms were loaded with x direction tensile strain. The strain of each step was 0.001. The graphene model was selected to achieve stable relaxation step size. The strain was applied continuously until the graphene film was destroyed.
(3) Tensile simulation of graphene in y direction. The method is the same as that in x direction, but the carbon atoms at the lower end of the film are fixed first, and the tensile strain load in y direction is applied to the upper carbon atoms.

2.3 Simulation Method Based on Short and Long Time Memory Neural Network

Long and short term memory (LSTM) neural network is an improved recurrent neural network (RNN) [7]. The long-term and short-term memory neural network is used to store all the information of the tensile mechanical properties of graphene during the simulation process. The data structure of the memory graphene tensile mechanical properties is shown in Fig. 2.

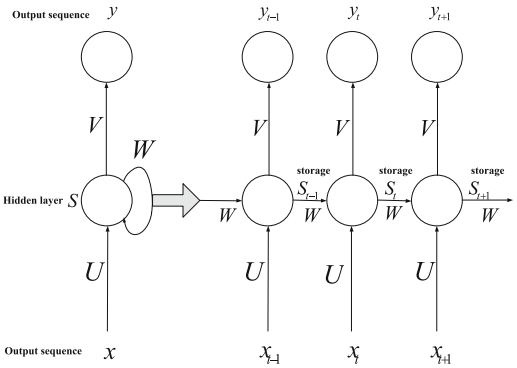


Fig. 2. Data structure diagram of tensile mechanical properties of long and short-term memory neural network memory graphene

In Fig. 2, t represents the long-term and short-term memory neural network, and the time step of storing data, i.e. $t = 1, 2, 3, \cdots$. x_t represents the input in step t, and V, U and W represent the hidden layer position of long and short memory neural network respectively. s_t is the memory unit, which is the state of the t time step of the hidden layer. If the state of the hidden layer W_{x_t} in the previous step is combined with the output U_{x_t} of the current input layer, the calculation formula of s_t is as follows:

$$s_t = f\left(U_{x_t} + W_{x_t} - 1\right) \tag{1}$$

In formula (1), f represents the nonlinear activation function, and y represents the output at the t time step.

According to the long and short-term memory neural network memory graphene tensile mechanical properties data structure diagram shown in Fig. 2, the results of each experiment are directly input into the long and short-term memory neural network architecture diagram, and all the experimental data can be analyzed and sorted, get the simulation result.

2.4 Tensile Mechanical Properties of Simulated Graphene

According to the Mermin-Wagner theory, long-wavelength fluctuations will destroy the long-range order characteristics of the two-dimensional crystal; at the same time, it can be known from the elastic theory that the stability of the two-dimensional film

is relatively poor when the effective temperature is greater than 0K, and it is especially prone to bending Phenomenon [8]. Therefore, in the past, scientists believed that "a perfect two-dimensional crystal structure can only exist stably under absolute zero conditions." However, the successful preparation of single-layer graphene broke this argument. Single-layer graphene can exist stably in the external environment of non-absolute zero degrees, which is related to the relaxation characteristics of graphene [9, 10]. Therefore, the study to simulate the tensile mechanical properties of graphene will first analyze the relaxation characteristics of the graphene model established this time, and then analyze the tensile mechanical properties of the graphene in the direction and direction.

2.4.1 Relaxation Properties of Graphene

Based on the experimental process, the graphene model shown in Fig. 1 is treated with unconstrained relaxation, and the total energy change curve of graphene in the relaxation process is obtained, as shown in Fig. 3.

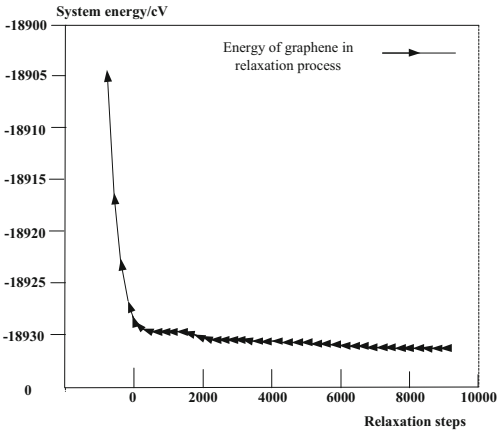


Fig. 3. Graphene total energy change curve during relaxation

It can be seen from Fig. 3 that when the number of simulation steps reaches 1000, the total energy of graphene has basically stabilized. When the number of simulation steps exceeds 2000, the total energy of graphene almost does not change, that is, the total energy of graphene reaches an equilibrium state. Judging from the energy stability, we think that the graphene monolayer is in a relatively stable state.

2.4.2 Stretching Simulation of Graphene in the *x* Direction

According to the previous section, the full unconstrained relaxation of graphene model is carried out to simulate and analyze the stable process of graphene. The number of relaxation steps for full unconstrained relaxation of graphene model is determined as 1000 steps. The tensile mechanical properties of graphene were simulated under 1000

step relaxation. Based on the above research process, the simulation process of tensile mechanical properties of graphene is determined. For the tensile simulation of graphene in x direction, the experimental results are shown in Fig. 4.

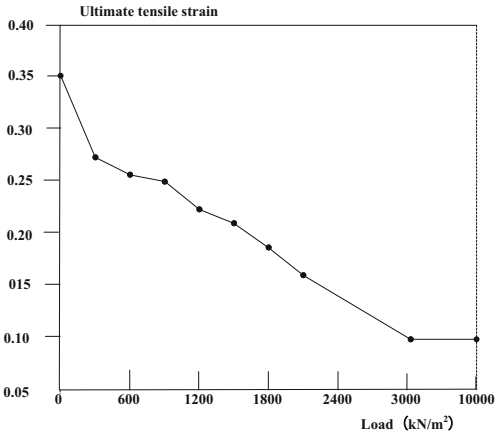


Fig. 4. Tensile simulation of graphene in the x direction

It can be seen from Fig. 4 that when graphene is stretched in the x direction to simulate the tensile mechanical properties of graphene, its initial tensile ultimate strain is 0.35. When the load is increased to 2000 kN/m^2, the tensile strength of graphene is the ultimate strain drops sharply, and the downward trend slows down as the load increases. When the load increases to 3000 kN/m^2, the resulting tensile strain no longer changes, indicating that the graphene film has been stretched under the action of the load. damage. It can be seen that in the x direction, the tensile graphene can withstand a maximum load of 3000 kN/m^2, and the tensile ultimate strain that can be withstood is 0.089.

2.4.3 Stretching Simulation of Graphene in the *y* Direction

Based on the tensile simulation of x direction, the mechanical properties of y direction tensile simulation were studied. At the same time, the tensile mechanical properties of graphene were simulated under 1000 step relaxation state. Based on the above research process, the simulation process of tensile mechanical properties of graphene is determined. For the tensile simulation of graphene in y direction, the experimental results are shown in Fig. 5.

It can be seen from Fig. 5 that the tensile graphene in the y direction simulates the tensile mechanical properties of graphene. As the load increases, the tensile strain of the graphene continues to decrease. When the load increases to 1800 kN/m^2 When the load reaches 3000 kN/m^2, the tensile strain of graphene has stopped changing and the film ruptures. It can be seen that in the y direction, the tensile graphene can withstand a maximum load of 3000 kN/m^2, and the tensile ultimate strain that can withstand is 0.117.

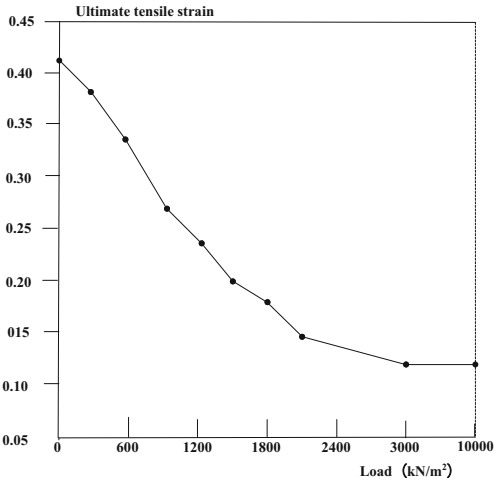


Fig. 5. Tensile simulation of graphene in direction *y*

2.5 Analysis of Tensile Mechanical Properties of Graphene

In this simulation, the tensile mechanical properties of graphene were studied. The tensile limit strain of graphene was studied by tensile simulation in *x* direction and *y* direction respectively. The tensile limit strain of graphene can be obtained under the action of load.

Before the simulation study, graphene was fully unconstrained relaxation to determine the stability of graphene itself and the energy change of graphene itself. According to the experimental results shown in Fig. 3, the relaxation step length of graphene is determined to be 1000 steps. From this, it can be judged that the relaxation results of graphene itself can affect the simulation results of the tensile mechanical properties of graphene. Only according to the relaxation step length of graphene and let the graphene reach an energy stable state can the tensile limit of graphene be obtained.

In the process of simulation, the long-term and short-term memory neural network is used to store and iterate the experimental data and the information before and after the simulation data, so as to determine the validity of the simulation research data. The experimental data shown in Fig. 4 and Fig. 5 are converted into the simulation data table of tensile mechanical properties of graphene, as shown in Table 1.

It can be seen from Table 1 that under this simulation study, the simulation data obtained show that the tensile force of graphene under load has no significant difference in direction *x* and direction *y*, but there is a certain difference in the ultimate tensile force that graphene can bear. Under the same load conditions, the young's modulus, tensile strength and ultimate strain of graphene in *x* direction are higher than those in *y* direction. It can be inferred that graphene has the phenomenon of non-uniform tensile force, which can bear different degrees of tensile force in different directions.

Since the graphene model used in this study is not perfect graphene, it has a perfect two-dimensional crystal structure, and there is no change in the structure in all directions. Therefore, it is inferred that the tensile strength of graphene is related to the atomic

Table 1. Simulation data of tensile mechanical properties of graphene.

Stretching direction	Load (kN/m^2)	Young's modulus/GPa	Tensile strength/GPa	Ultimate tensile strain
x direction	0	1033.75	200.68	0.409
	300	983.12	190.04	0.380
	600	947.44	170.47	0.336
	900	918.50	138.60	0.271
	1200	907.21	126.38	0.239
	1500	875.23	112.05	0.200
	1800	829.55	104.24	0.178
	2100	786.99	89.38	0.144
	3000	743.48	74.89	0.117
y direction	0	977.05	188.93	0.349
	300	946.13	174.01	0.270
	600	915.84	166.16	0.254
	900	897.73	161.43	0.250
	1200	865.32	142.53	0.220
	1500	837.58	131.09	0.207
	1800	843.70	114.26	0.183
	2100	788.00	97.26	0.156
	3000	732.42	59.57	0.089

distance of the graphene itself, and the amount of matter will also affect the tensile strength of graphene.

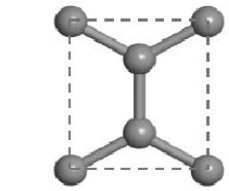
In summary, the tensile mechanical properties of graphene will be affected by factors such as its structure, material atoms, and the distance between atoms, and there will be differences in the tensile force that can be withstood in different directions.

3 Experiment and Analysis

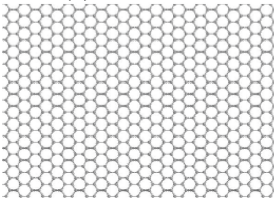
In order to verify the simulation method of tensile mechanical properties of graphene, zigzag graphene was selected as the research object of this experiment. Lamps was used as graphene modeling software. ANSYS motion mechanical simulation software was selected as the operation software of the simulation experiment. The simulation method of tensile mechanical properties of graphene in this study was recorded as experimental group A; the two simulation methods of tensile mechanical properties of graphene mentioned in the literature were recorded as group B and group C respectively. The experimental object and the experimental environment were determined. The stress-strain curves and tensile mechanical properties of graphene were compared among the three groups of simulation methods, and the results were in error with the experimental values.

3.1 Experiment Preparation

The sawtooth graphene selected in this experiment uses the lattice command in the LAMMPS modeling software to establish a sawtooth graphene model, as shown in Fig. 6.



(a) Basic unit



(b) Hexagonal lattice structure

Fig. 6. Sawtooth graphene model

The zigzag graphene model shown in Fig. 6 is a honeycomb 2-D crystal composed of single-layer hexagonal cell carbon atoms. The length of carbon carbon bond is about 0.142 nm, the thickness is 0.335 nm, the number of atoms is 15134, and the size is 19.8839 nm * 19.6800 nm.

According to the experimental objects selected in this experiment, ANSYS motion mechanical simulation software was used to simulate the tensile mechanical properties of serrated graphene model according to three groups of tensile mechanical simulation methods. The experimental environment for its operation is shown in Table 2.

Table 2. Experimental environment.

Lab environment	Configuration	Configuration
Software environment	Drive	Ubuntu 16.04 LTS (64bit)
	Neural network framework	TensorFlow0.12、Keras1.2
Hardware environment	Processor	Intel i7–7700 CPU 3.60 GHz
	RAM	8 GB
	Graphics card model	NVIDIA GeForce GTX 1060
	Graphics card memory	6 GB

According to the experimental parameters set by the selected experimental objects, three groups of graphene tensile mechanical properties simulation methods were used to simulate the selected graphene in this experiment, and the simulation results of the three groups of methods were compared.

3.2 The First Set of Experimental Results

Based on the experimental parameters designed for this experiment, the first set of experiments was carried out. Three sets of mechanical performance simulation methods were used to simulate this experiment respectively. The sawtooth graphene model shown in Fig. 6 was established using the sawtooth graphene to obtain the graphene stress-strain curve. The graphene stress-strain curves simulated by the three sets of simulation methods were compared with the graphene stress-strain curves obtained from experiments, and the simulation results of graphene tensile mechanical properties were obtained, as shown in Fig. 7.

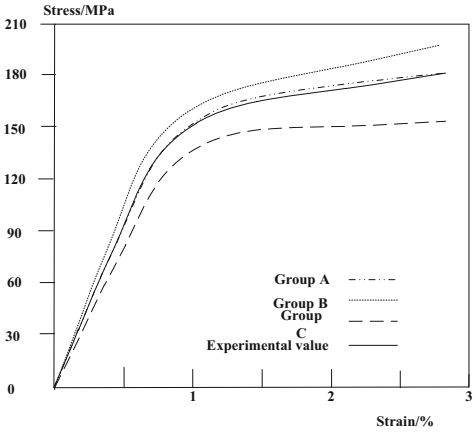


Fig. 7. Comparative analysis of stress-strain curves between simulation and experiment

It can be seen from Fig. 7 that the graphene stress-strain curve obtained in experiment C group is obviously smaller than the experimental value, and there is a gap between the simulated tensile mechanical properties of graphene and the experimental value; the graphene stress obtained in experiment B group is − The strain curve is obviously larger than the experimental value, and there is a gap between the simulated tensile mechanical properties of graphene and the experimental value; experimental group A simulates the tensile mechanical properties of graphene, and the graphene stress-strain curve obtained is very close to the experimental value, and the coincidence rate of experimental results is extremely high. It can be seen that the simulation results of the graphene tensile mechanical properties simulation method studied in this study have extremely high accuracy, which can be used as tensile mechanical properties and stress-strain curve experimental results.

3.3 The Second Group of Experimental Results

On the basis of the first group of experiments, the second group of experiments was carried out. The elastic modulus, tensile strength and ultimate tensile strain of the first group of graphene Tensile Mechanical Properties Simulation and experiment were extracted. Compared with three groups of simulation methods, the numerical simulation results of graphene tensile mechanical properties in the experimental process. The analysis results of tensile mechanical properties of graphene by three groups of simulation methods are judged, as shown in Table 3.

Table 3. Tensile Properties of serrated graphene.

Property method	Experimental value	Group A	Group B	Group C
Elastic model/GPa	174	174	165	155
Tensile strength/GPa	90	87	86	84
Ultimate tensile strain	0.353	0.348	0.335	0.332

It can be seen from Table 3 that the simulated value of the tensile mechanical properties of graphene obtained in the experiment group C differs the most from the experimental value; the gap between the simulated value of the simulated tensile mechanical properties of the graphene in experiment group B and the experimental value Although it is stronger than the experimental group C, there is a large gap between the experimental value; and the tensile mechanical properties of the graphene obtained in the experimental group A are closer to the experimental value, only the difference in tensile strength is 3 GPa and the ultimate tensile strength. The tensile strain, the difference is 0.005, is obviously stronger than the experimental group B and the experimental group C. It can be seen that the tensile mechanical properties of graphene obtained by the simulation method of graphene tensile mechanical properties in this study can be used as experimental results.

Based on the above two groups of experiments, it can be seen that the simulation results obtained by the simulation method of graphene tensile mechanical properties are very close to the experimental results, which can be used as the experimental results.

3.4 Experimental Results of the Third Group

Based on the above experimental, in order to comprehensively compare the comprehensive properties of different methods, the simulation time of graphene tensile mechanical properties was compared, and the results are shown in Table 4.

Analysis of Table 4 shows that the experimental group A graphene tensile mechanical properties of simulation time average of 0.57 s, the experimental group B graphene tensile mechanical properties of simulation time average of 1.59 s, the experimental group C graphene tensile mechanical properties of simulation time average of 1.70 s, compared with the experiment group B and group C, the experimental group A simulation time is shorter, simulation shows the method of graphene the stretch mechanics performance is more efficient.

Table 4. Comparison of simulation time (unit:s)

Number of experiments	Group A	Group B	Group C
1	0.36	1.42	2.01
2	0.56	1.56	1.96
3	0.58	1.78	1.58
4	0.62	1.57	1.63
5	0.66	1.48	1.75
6	0.57	1.63	1.95
7	0.49	1.62	1.47
8	0.63	1.28	1.25
9	0.61	1.57	1.47
10	0.58	1.98	1.96
Average	0.57	1.59	1.70

4 Concluding Remarks

To sum up, the study of graphene tensile mechanical properties simulation method, give full play to the advantages of long-term and long-term memory neural network for data memory and iterative ability, and improve the accuracy of simulation experiment results. However, the simulation method of tensile mechanical properties of graphene in this study did not consider the graphene with different shapes and structures, and the tensile mechanical properties obtained would have certain differences, which would have a certain impact on the research results of tensile mechanical properties of graphene. Therefore, in the future research, it is necessary to further study the simulation method of tensile mechanical properties of graphene, taking into account the shape and structure of graphene itself, so as to ensure the preciseness of simulation results and further improve the simulation accuracy.

Acknowledgments. Teaching Quality and Teaching Reform Project of Guangdong Undergraduate Colleges and Universities: Construction Project of Experiment Demonstration Center (2017002).

References

1. Gao, H., Xu, J.: Numerical study on aerodynamic performance of three-dimensional flapping wing. Comput. Simul. **37**(6), 36–39,151 (2020)
2. Han, Z., Zou, L., Xin, Z., et al.: Molecular dynamics simulation of vital physical properties of epoxy/carbon nanotube composite coatings on DC GIL insulators. Trans. China Electrotech. Soc. **33**(20), 4692–4703, 4721 (2018)
3. Li, J.J., Lu, B.B., Xian, Y.H., et al.: Characterization of nanoporous silver mechanical properties by molecular dynamics simulation. Acta Physica Sinica **67**(5), 226–234 (2018)

4. Liu, S., Lu, M., Li, H., et al.: Prediction of gene expression patterns with generalized linear regression model. Front. Genet. **10**, 120 (2019)
5. Yao, X., Wang, X., Wang, S.H., et al.: A comprehensive survey on convolutional neural network in medical image analysis. Multimedia Tools Appl., 1–45 (2020)
6. Liu, S., Bai, W., Zeng, N., et al.: A fast fractal based compression for MRI images. IEEE Access **7**, 62412–62420 (2019)
7. Huang, S.: Mechanical properties of hydrated calcium silicate simulated by molecular dynamics. Bull. Chin. Ceramic Soc. **37**(5), 1687–1692 (2018)
8. Fu, K., Wang, G., Wang, S., et al.: Simulation and analysis of mechanical properties of bilayered all-ceramic denture. Shandong Sci. **31**(5), 31–37, 88 (2018)
9. Zhang, C., Zhao, X., Fu, X., et al.: Progress in the application of molecular dynamics simulation in the study of physical and chemical properties of propellant components. Chin. J. Explos. Prop. **41**(6), 531–542 (2018)
10. Zheng, C., Cui, Z., Huang, Y.: Simulation of microstructures and mechanical properties of ternary polymer blends. J. Func. Polymers **31**(4), 305–314 (2018)