E3S Web of Conferences **573**, 02001 (2024) https://doi.org/10.1051/e3sconf/202457302001
SDER 2024

The Variation Law of CO_2 Adsorption / Desorption Energy of Coal under Infrared Action

Kai Ma[1,2]

[1]China Coal Technology and Engineering Group Chongqing Research Institute, Chongqing 400037, China
[2]State Key Laboratory of Coal Mine Disaster Prevention and Control, Chongqing 400037, China

Abstract: The adsorption / desorption process of coalbed methane is actually a process of mutual transformation between free state and adsorbed state of gas molecules. Because the molecular movement process is inevitably accompanied by energy changes, it is of great significance to study the energy changes in the process of CO_2 adsorption / desorption of coal to study the migration law of coalbed methane. The adsorption and desorption characteristics of CO_2 on coal under different infrared powers were studied by using the self-designed infrared isothermal adsorption / desorption simulation tester. The energy calculation theory in the adsorption / desorption process was used to obtain the energy change law in the adsorption / desorption process under the experimental conditions. The results show that the CO_2 adsorption / desorption efficiency of coal under the action of power infrared can be explained from the energy point of view, and the free energy of the adsorption and desorption state is affected by the infrared power and pressure, which is consistent with the experimental results of CO_2 adsorption / desorption of coal under the action of power infrared. The adsorption characteristic curves of different infrared powers have basically the same change trend, which all meet the cubic polynomial fitting relationship, and the fitting degree is high, R^2 is above.

1. Introduction

As a clean energy, coalbed methane is a renewable resource. It mainly occurs in coal seams and their surrounding rocks, and is an unconventional natural gas. Although China's coalbed methane resources are very rich, due to geological differences, coalbed methane occurrence conditions are relatively poor. Low reservoir pressure, low coal permeability and low adsorption saturation are the objective factors that lead to low efficiency of coalbed methane exploitation. Due to the above many factors, coalbed methane desorption and migration are difficult, resulting in the current situation of low production and rapid production decline of most coalbed methane wells in China. Based on the above situation, it is one of the important work to study the adsorption / desorption characteristics of coalbed methane in the reservoir to improve its mining efficiency.

The adsorption of CO_2 by coal is a complex physical process. Due to the different microscopic pore structure of coal and the different energy changes in the macroscopic adsorption / desorption process, the adsorption / desorption capacity of CO_2 by coal is different. The essence of adsorption is a spontaneous trend of coal to reduce surface free energy by reducing surface tension. Therefore, the study of energy changes in the process of CO_2 adsorption by coal can essentially explain different adsorption phenomena[1-7]. Liu et al.[8] studied the variation law of coal energy with different coal structure in the process of isothermal adsorption. Liu Jikun[9] conducted an experimental study on the thermal effect of coal gas adsorption and desorption process. Wu Di et al[10] studied the desorption law of gas in briquette under ultrasonic thermal effect. Lu et al.[11] conducted an experimental study on the influence of thermal effect of cavitation water jet on coal permeability. In order to improve the mining efficiency of coalbed methane and increase the output of coalbed methane, it is very important to study new coalbed methane mining methods. The research group proposed a new method of using power infrared to exploit coalbed methane. Therefore, in the process of coalbed methane exploitation, the study of the change law of CO_2 adsorption / desorption energy of coal under the action of power infrared is an important basis for the follow-up study of coalbed methane exploitation by power infrared. The energy variation law of coal adsorption / desorption process under different infrared power and different pressure was studied by using the self-designed power infrared isothermal adsorption / desorption simulation tester. The test results have a positive effect on the targeted development of coalbed methane mining efficiency and productivity prediction research.

*Corresponding author: makai0810@163.com

2. Infrared isothermal adsorption /desorption experiments

2.1. Experimental installation

The radiation effect of electromagnetic wave mainly depends on the degree of absorption of electromagnetic wave by the medium. The higher the absorption rate, the better the radiation effect. The absorption rate depends on the type and surface state of the heated material. Due to the special physical properties of coal, it has good absorption performance for electromagnetic waves. In this experiment, the self-designed electromagnetic wave adsorption / desorption simulation test instrument was used to carry out the experiment. The experimental instrument was mainly composed of electromagnetic wave generator, constant temperature box, sample cylinder, reference cylinder, data acquisition device and high pressure gas cylinder. The allowable electromagnetic wave radiation power of the device is 0~100W, and the allowable experimental pressure is 0~20MPa. The experimental principle of isothermal adsorption / desorption of coalbed methane under the action of electromagnetic wave is as follows: Using the compression factor state equation, the total gas amount n0 at the initial time is obtained. The balance valve was opened. After the sample was fully adsorbed, the residual gas amount n1 and the adsorption amount $n= n_0-n_1$ were obtained by using the compression factor gas state equation. The calculation principle of desorption amount is the same as that of the above adsorption amount. The simulation test device of isothermal adsorption / desorption of coalbed methane based on power infrared is shown in Fig.1.

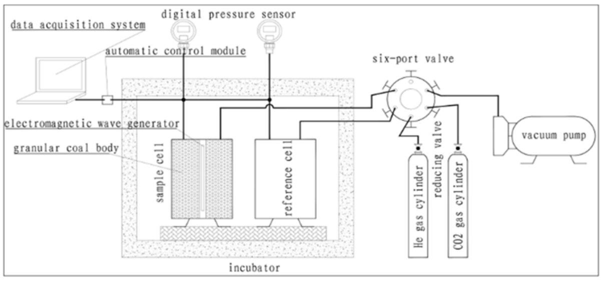

Fig.1 Simulation of Coal bed Methane Isothermal Adsorption / Desorption Simulator Based on Power Infrared

2.2. Experimental installation

The experimental coal sample is taken from the experimental sample of Haizhou mine. The gas measured in the free space volume is high-purity helium (99.99% purity), and the gas adsorbed and desorbed in the experiment is high-purity CO_2 gas (99.99% purity). The coal rock parameters selected in the experiment are shown in Table 1.

Table 1 the Coal Rock Parameters Selected in the Experiment

component	organic carbon	clay minerals	vitrine group	others
content (%)	75.00	10.28	6.22	8.50

2.3. Experimental result

The experimental results of adsorption / desorption of CO_2 by coal rock under different infrared power are shown in Table 2.

Table 2 Coal for Power at Different Infrared CO_2 Adsorption / Desorption Results

state	infrared power P_{IP} (W)	Langmuir volume V_L (cm³/g)	Langmuir pressure P_L (Mpa)
adsorption	15	39.76540	2.921
	20	36.67974	2.919
	25	31.47020	2.919
	30	25.74953	2.999
desorption	15	41.09540	2.314
	20	37.43388	2.434
	25	33.68138	2.648
	30	27.32070	2.600

3. Calculation of adsorption / desorption energy under infrared radiation

3.1. Infrared power-temperature conversion relationship

The temperature variation law of coal-rock mass under different far-infrared radiation power is the basis of this experiment. Firstly, the experiment on the temperature variation law of coal-rock mass under different far-infrared radiation power is carried out. Then, the obtained experimental data are fitted to obtain the following far-infrared radiation power-far-infrared action temperature conversion formula (Formula (1)).

$$T = 265.0217 + 3.56908 P_{IP} \tag{1}$$

In the formula : T is temperature, K ; P_{IP} is infrared power, W.

3.2. Surface free energy of coal adsorption

There are many pores in the coal rock mass. At the micro molecular motion level, due to the vacancy of the carbon atom on the surface of the pore, the force on both sides of the carbon atom is unbalanced, resulting in the traction force moving towards the inside of the coal body, so that the carbon atom has the tendency to move towards the inside of the coal rock mass. Under this gravitational trend, the energy obtained by the carbon atom on the surface of the coal rock mass moving towards the inside of the coal rock mass is the surface free energy. The calculation method of surface free energy in the process of carbon dioxide adsorption by coal rock mass can be expressed as Equation (2).

$$\Delta\gamma = \frac{V_L RT}{V_0 S} \ln(1 + \frac{P}{P_L}) \tag{2}$$

In the formula : V_L represents Langmuir volume ; P_L represents Langmuir pressure; P represents CO_2 pressure; $\Delta\gamma$ represents the reduction value of free energy on the surface of coal and rock mass, J/m^2; R is the universal gas constant, 8.3145J/(mol·K) ; V_0 represents the molar volume of gas under standard conditions, 22.4 L/mol ; S represents the specific surface area of coal, m^2/g.

After differentiating the variable pressure P in equation(2), and then substituting equation(1) into it, the change value of free energy of coal and rock mass wall at each pressure point is obtained. The relationship is shown in equation(3).

$$\Delta\gamma_p = \frac{V_L R(265.0217+3.56908P_{IP})P_L}{V_0 S(P_L+P)} \quad (3)$$

3.3. Coal adsorption potential and adsorption space

When the pressure at the adsorption equilibrium of the gas medium is P_i, the pressure of the adsorption layer on the surface of the coal rock matrix is the saturated adsorption pressure P_0 of the gas medium. According to the theory of thermodynamics, the energy required for each gram of gas medium to change from the free state to the adsorption state is calculated by Equation (4).

$$\varepsilon = \int_{p_i}^{P_0} \frac{RT}{P} dP = RT\ln\frac{P_0}{P_i} = R(265.0217+3.5608P_{IP})\ln\frac{P_0}{P_i} \quad (4)$$

In the equation, ε is the adsorption potential, J/mol ; P_0 is the gas saturated steam pressure, MPa ; P_i is the equilibrium pressure of the ideal gas at constant temperature, MPa ; P is the equilibrium pressure, MPa ; R is a universal gas constant, J/(mol·K); T is the absolute temperature, K.

The critical state CO_2 saturated vapor pressure under this experimental condition refers to the pressure value of the vapor when it is in phase equilibrium with the coal rock mass under a certain infrared power in a closed condition.

The pressure P_0 of the adsorption layer on the surface of the coal rock matrix is calculated by Equation (5).

$$P_0 = P_c\left(\frac{T}{T_c}\right)^2 = P_c\left(\frac{265.0217+3.56908P_{IP}}{T_c}\right)^2 \quad (5)$$

In the formula : P_c is the critical pressure of carbon dioxide, with a value of 7.38MPa ; Tc is the critical temperature of carbon dioxide, with a value of 221.7K.

The pore structure of coal and rock mass is characterized by the adsorption space volume. The space volume occupied by the adsorption of CO_2 gas medium in the pores of coal rock is calculated according to Equation (5).

$$\omega = \frac{V_{ad}M}{\rho_{ad}} \quad (6)$$

In the equation : ω for the adsorption space volume, m^3/t ; M is the gas molecular weight, g/mol ; V_{ad} is the amount of gas adsorption, mol/g ; A_d is the density of CO_2 gas adsorption phase, which is 1.40928 g/m^3.

4. Analysis of adsorption / desorption energy calculation results

Fig.2 and Fig.4 are the total free energy reduction curves of different infrared power adsorption states and desorption states, respectively. Fig.3 and Fig.5 are the free energy reduction curves of different infrared power adsorption states and desorption states at each pressure point, respectively. Fig.6 to Fig.9 are the adsorption characteristic curves at far infrared power of 15W, 20W, 25W and 30W, respectively. Fig.10 is the adsorption potential change curve of different states, and Table 3 is the adsorption characteristic curve fitting data table.

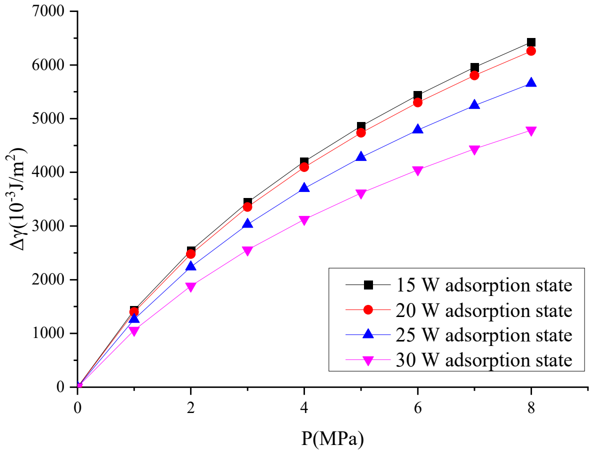

Fig.2 the Total Reduction Curve of Free Energy in Different Infrared Power Adsorption States

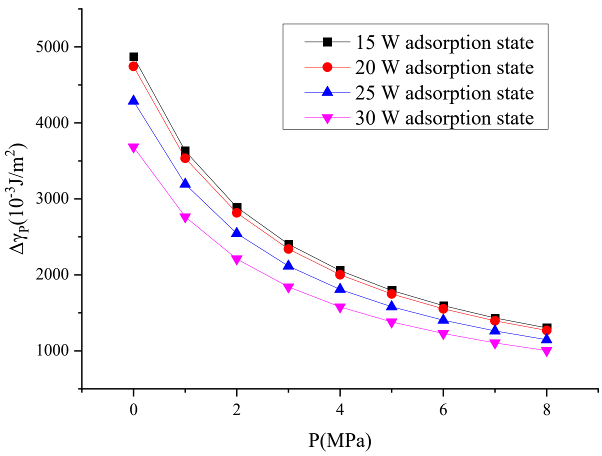

Fig.3 the Free Energy Reduction Curves of Each Pressure in Different Infrared Power Adsorption States

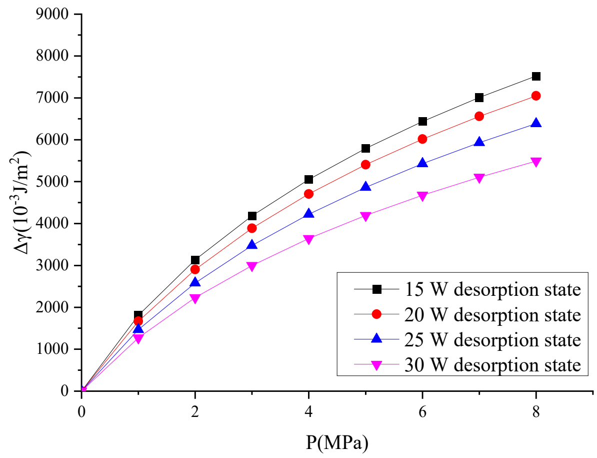

Fig.4 the Total Reduction Curve of Free Energy in Different Infrared Power Desorption States

https://doi.org/10.1051/e3sconf/202457302001

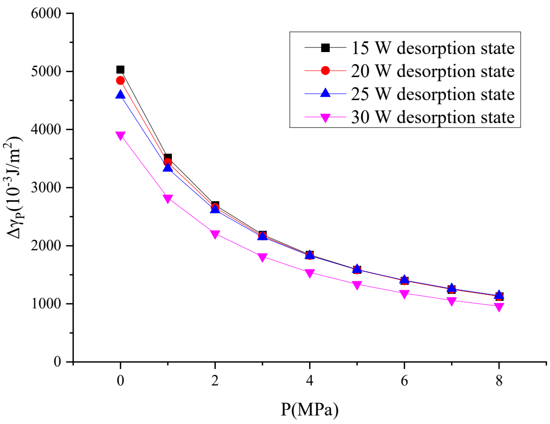

Fig.5 Free Energy Reduction Curves of Different Pressure in Different Infrared Power Adsorption States

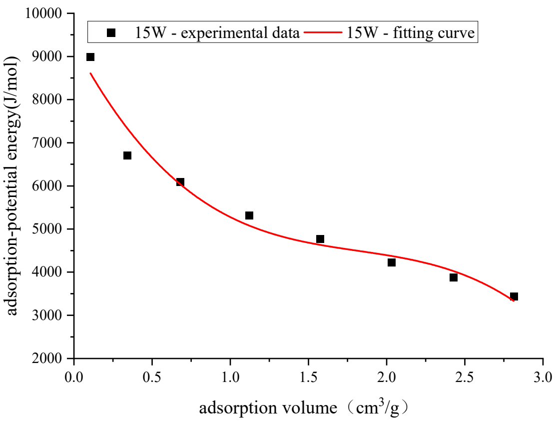

Fig.6 Adsorption Characteristic Curve of Infrared Power 15W

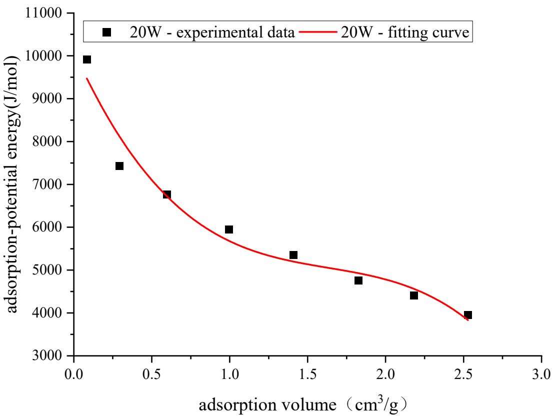

Fig.7 Adsorption Characteristic Curve of Infrared Power 20W

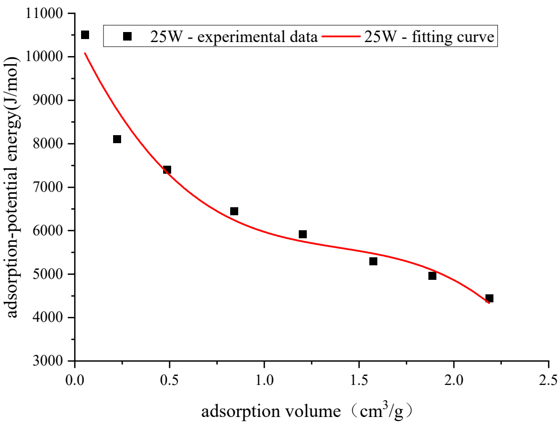

Fig.8 Adsorption Characteristic Curve of Infrared Power 25W

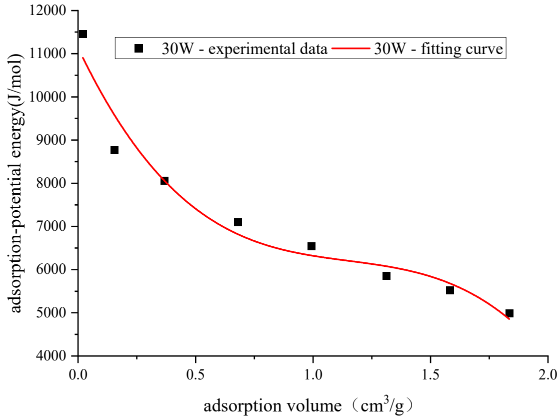

Fig.9 Adsorption Characteristic Curve of Infrared Power 30W

Table 3 Adsorption Characteristic Curve Fitting Data Table

power	Adsorption characteristics cubic curve fitting (ε=aω +bω^2+cω^3+d)				
	a	b	c	d	R^2
15W	-6871.9	3490.3	-640.3	9299.0	0.9
20W	-8095.7	4586.6	-936.7	10120.7	0.9
25W	-9252.1	6132.2	-1464.8	10557.0	0.9
30W	-11433.2	9316..8	-2697.8	11135.1	0.9

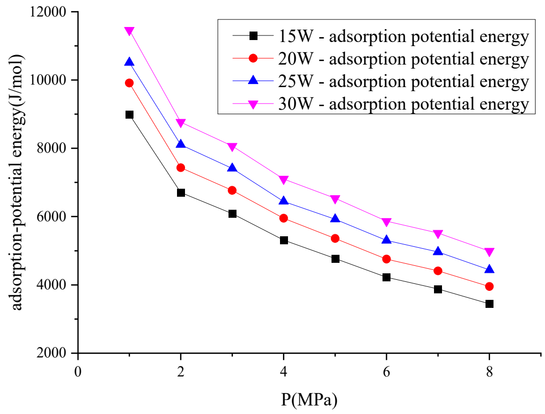

Fig .10 Adsorption Potential Curves in Different States

By comparing and analyzing the total reduction value of free energy, the reduction value of each pressure point and the adsorption characteristic curve in the process of CO_2 adsorption / desorption by coal under the action of power infrared, the following rules are obtained.

(1) Under the action of power infrared, the change trend of the total reduction of free energy in the process of CO_2 adsorption / desorption by coal is consistent. At the same infrared power, the total reduction of free energy increases with the increase of pressure. Under the same pressure condition, the total reduction of free energy decreases with the increase of infrared power. Temperature change is a macroscopic sign of molecular motion. The above conclusions show that with the increase of infrared power, the total free decrease of CO_2 molecules becomes smaller, and the kinetic energy of CO_2 molecules increases, which leads to the decrease of the adsorption capacity of coal to CO_2 molecules, thus improving the desorption efficiency. The pressure is positively correlated with the total reduction of free energy. In the process of increasing pressure, the kinetic energy of CO_2 molecules decreases, thus promoting the adsorption efficiency of CO2 molecules by coal. The

results are consistent with the macroscopic results of CO_2 adsorption / desorption by coal under the action of power infrared.

(2) The free energy reduction curve of each pressure point in different infrared power adsorption states reflects the reduction rate of total free reduction under different infrared power, and it is also a sign of the difficulty of coal adsorption of CO_2 under the action of infrared reaction power. Under the condition of the same infrared power, the decrease of free energy at each pressure point of CO_2 adsorption / desorption state decreases with the increase of pressure. It shows that the decrease rate of the total free energy decrease during the adsorption / desorption process becomes slower, and the coal is more difficult to carry out CO2 over time during the adsorption and desorption process.

(3) The adsorption potential energy decreases with the increase of adsorption space. The variation trend of adsorption characteristic curves of different infrared powers is basically the same, which satisfies the cubic power function fitting relationship, and the fitting degree is high, and R^2 is above 94 %.

(4) Under the same pressure, the adsorption potential increases with the increase of power when the free state of CO_2 becomes the adsorbed state under the action of power infrared. It shows that the higher the infrared power is, the more work CO_2 does from free state to adsorption state, and the more difficult it is for coal to adsorb CO_2. Under the same infrared power condition, the adsorption potential is negatively correlated with the pressure.

5. Conclusion

(1) The rate and difficulty of CO_2 adsorption / desorption by coal under the action of power infrared are related to the total reduction of free energy and the reduction of free energy at each pressure point. The greater the total reduction of free energy and the reduction of free energy at each pressure point, the easier it is to be adsorbed and the higher the adsorption efficiency.

(2) The variation trend of adsorption characteristic curves of different infrared powers is basically the same, which satisfies the cubic power function fitting relationship, and the fitting degree is high, and R^2 is above 94 %.

(3) The CO_2 adsorption / desorption efficiency of coal under the action of power infrared can be explained from the energy point of view. The free energy of adsorption and desorption state is affected by infrared power and pressure. This result is consistent with the experimental results of CO_2 adsorption / desorption by coal under the action of power infrared.

Reference

1. Shi R, Liu J S, Wei M Y, et al. Mechanistic analysis of coal permeability evolution data under stress-controlled conditions[J]. International Journal of Rock Mechanics and Mining Sciences, 2018, 110: 36-47.
2. Yang, D., Sarhosis, V., Sheng, Y. Thermal–mechanical modelling around the cavities of underground coal gasification[J]. Journal of the Energy Institute, 2014, 87(4): 321-329.
3. Liang Yunpei, Lv Xuewei, Luo Yongjiang, et al. study on the response of gas adsorption and desorption characteristics of Xinjiang difficult-to-mine coal seam to soluble organic matter[J]. Mining Safety & Environmental Protection, 2024,51(01):43-50.
4. Lin Haifei, Chen Chen, Long Hang, et al. Study on effect of temperature on gas flow and coal deformation in whole process[J]. China Safety Science Journal,2023,33(08):59-67.
5. Tang Xiaoyan, Chen Xinyi, Zheng Leiqing, et al. Review of Conductive Characteristics of Gas-bearing Coal[J]. Science Technology and Engineering,2023,23(25):10617-10624.
6. Zheng Chao, Ma Dongmin, Chen Yue, et al. research progress on response law of adsorption / desorption microscopic characteristics of coalbed methane to water content of coal and rock mass [J]. Coal Science and Technology,2023,51(02):256-268.
7. Zhong Qianghua, Jane Miaofu. The Simulation of the Thermal Analysis Process of Dicalcium Silicate Solid-state Reaction [J]. Non-Metallic Mines,2014,37(01):31-33.
8. Liu Shanshan, Meng Zhaoping. Study on energy variation of different coal-body structure coals in the process of isothermal adsorption [J]. Journal of China Coal Society,2015,40(06):1422-1427.
9. Liu Jikun. Experimental study on thermal effect of coal gas adsorption and desorption process [D]. china university of mining &technology- beijing,2012.
10. Wu Di, Xu Jun, Xiao Xiaochun, et al. Experimental study on gas desorption regularity of briquette coal under ultrasound thermal effect [J]. Journal of Safety Science and Technology,2015,11(10):5-10.
11. Lu Yiyu, Ding Hong, Ge Zhaolong, et al. Experiment study of effect of coal permeability under thermal effect of cavitation water jets [J]. Rock and Soil Mechanics,2014,35(05):1247-1254.