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The mechanisms of gas generation during coal deformation: Preliminary observations

RongTing Xu [a,b], HuiJun Li [a,b,c], ChenChen Guo [d], QuanLin Hou [a,b,*]

[a] Key Lab of Computational Geodynamics, Chinese Academy of Sciences, Beijing 100049, China
[b] College of Earth Sciences, University of Chinese Academy of Sciences, Beijing 100049, China
[c] Yunnan Copper Sanmu Mining Industry Co. Ltd., Yunnan 650000, China
[d] School of Chemistry and Chemical Engineering, University of Chinese Academy of Sciences, Beijing 100049, China

HIGHLIGHTS

- Deformation experiments of coal were designed to explore the mechanisms of gas generation.
- CO was generated during these experiments.
- The energy required for CO generation was also calculated using quantum chemistry methods.

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ABSTRACT

Gas generation often occurs during high-temperature and high-pressure deformation experiments on coal. In this work, sub-high-temperature and sub-high-pressure deformation experiments on coal were designed to explore the mechanisms of gas generation during coal deformation. The coal samples for coal deformation experiments were anthracite coals collected from the Qudi Mine in the Southern Qinshui Basin of China. The coal samples showed obvious ductile deformation and CO was generated at a temperature of 200 °C, pressure of 75 MPa and strain rate of 10^{-5} s^{-1}. The energy required for CO generation could be calculated by quantum chemistry methods and mechanical energies during these experiments were also calculated. The calculated results suggested that mechanical energy transforms into strain energy during the deformation of coal, and strain energy can promote the deformation and breakage of the coal's molecular units, resulting in deformation energy accumulation of dislocation and creep in the coal's interior nucleus. Upon accumulation of strain energy, the coal's molecular structure deforms by breaking old bonds and forming new ones, resulting in CO generation.

1. Introduction

Coal and gas outbursts always occur in tectonic deformation coals (i.e. tectonic coals) of fault or shear zones. The damaged degree of tectonic coals is an important indicator for measuring the danger of coal and gas outbursts. Intense shear zones, especially mylonitic coal areas, are consistently prone to coal and gas outbursts [1–4]. Tectonic coals studies have been carried out by many researchers. For example, Cao et al. [5] found that dynamic metamorphism is a type of function that deforms coal and reforms its physical and chemical structure. Dynamic metamorphism can promote chemical activity in coals, thus resulting in stress polycondensation and stress degradation [6]. Cao et al. [7] conducted an experiment using tectonic coal and primary structure coal of the same rank. These results showed that the former had a higher number of chloroform extracts than the latter. Furthermore, they stated that tectonic deformation would most likely impact the hydrocarbon generation of coals. Pan et al. [8] studied the different tectonically deformed coals and investigated that the tectonic deformation has an obvious effect on the coal methane adsorption capacity at low temperature. Hou et al. [4,9] found distinct differences in the energy transformation mechanisms of dynamic metamorphism under different deformation mechanisms (brittle, ductile and transitional). Under brittle deformation conditions, the change in the chemical structure is caused by kinetic energy, which is transformed primarily by mechanical friction between fractures. Under ductile deformation conditions, the accumulated strain energy damages the chemical structure of the coal. Peters first stated the mechanochemical theory in 1962 and coal researchers have used this theory ever since that time [10]. Researchers have found that the process of organic matter

* Corresponding author at: Key Lab of Computational Geodynamics, Chinese Academy of Sciences, Beijing 100049, China. Tel.: +86 13910023465.

E-mail addresses: xurongting11@mails.ucas.ac.cn (R. Xu), huijun871@gmail.com (H. Li), guochenchen10@mails.ucas.ac.cn (C. Guo), quhou@ucas.ac.cn (Q. Hou).

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transformation, including the formation and transformation of hydrocarbon, required sufficient energy which could be produced by dynamic metamorphism [11,12].

Over the last 30 years, researchers have conducted a significant number of high-temperature and high-pressure deformation experiments on coal and have found that gas generation occurs during these processes [13,14]. Some coal samples have even burst with substantial gas emissions [15,16]. However, it should be noted that such experiments were performed in an open space; therefore, the gas could not be collected, and the temperature of the experiments reached the pyrolysis temperature of coal. Thus, the gas was not isolated from pyrolysis gas. To better understand whether there is a relationship between coal and gas outbursts and coal deformation and whether the outburst gases generated are due to changes within coal chemical structure, sub-high-temperature and sub-high-pressure deformation experiments on the coal were designed to study the mechanisms of gas generation during coal deformation.

2. Sample selection and experiments

2.1. Sample selection

To avoid influences from other factors during coal deformation experiments at different temperatures, pressure and strain rates, a whole coal sample (Qudi01) was collected from the Qudi Mine in the Southern Qinshui Basin of China. The anthracite coal with a vitrinite reflectance of 4.03%, maintaining its primary structure, was used. The anthracite sample was made for 10 cylinders, all of which had the same diameter (20 mm) and length (40 mm). All experimental samples were desorbed for more than 4 h at a pressure of 0.1 MPa, after that, which were vacuumized until no gas was collected from the samples. The size (height: 30 cm; length: 55 cm; width: 30 cm) of the anthracite sample is shown in Fig. 1, the ultimate, maceral analysis data of the anthracite sample are shown in Table 1.

2.2. Experiments

The experimental apparatus included a high-temperature and high-pressure gas medium triaxial test system, with argon as the gas medium. A YAMATAKE DCP30 temperature controller was used to control temperatures, and a digital hydraulic servo machine was used to control the axial pressure. The entire sample, tungsten carbide and a corundum column were all packaged in an annealing copper tube (Fig. 2) with a wall thickness of 0.35 mm. The two heads of the copper tube had an o-ring seal to isolate the gas medium and the sample. The area between the copper pipe and the heat furnace was filled with boron nitride powder, which was used for heat transfer and preventing gas convection. The experiment included a thermocouple channel and a vent connection gas collection device. The temperature of coal deformation experiments was 50–200 °C and pressure was 30–75 MPa. The strain rate was

Table 1
The Ultimate, maceral analysis of the anthracite sample.

Sample	Ultimate analysis (%)					Maceral analysis (%)		
	C	H	O	N	S	Vitrinite	Inertinite	Exinite
Qudi01	93.22	3.04	2.30	1.07	0.37	66.80	22.40	4.80

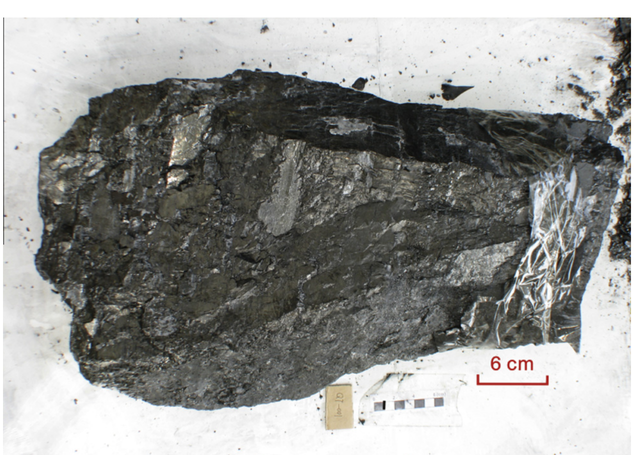

Fig. 1. The coal sample with primary structure.

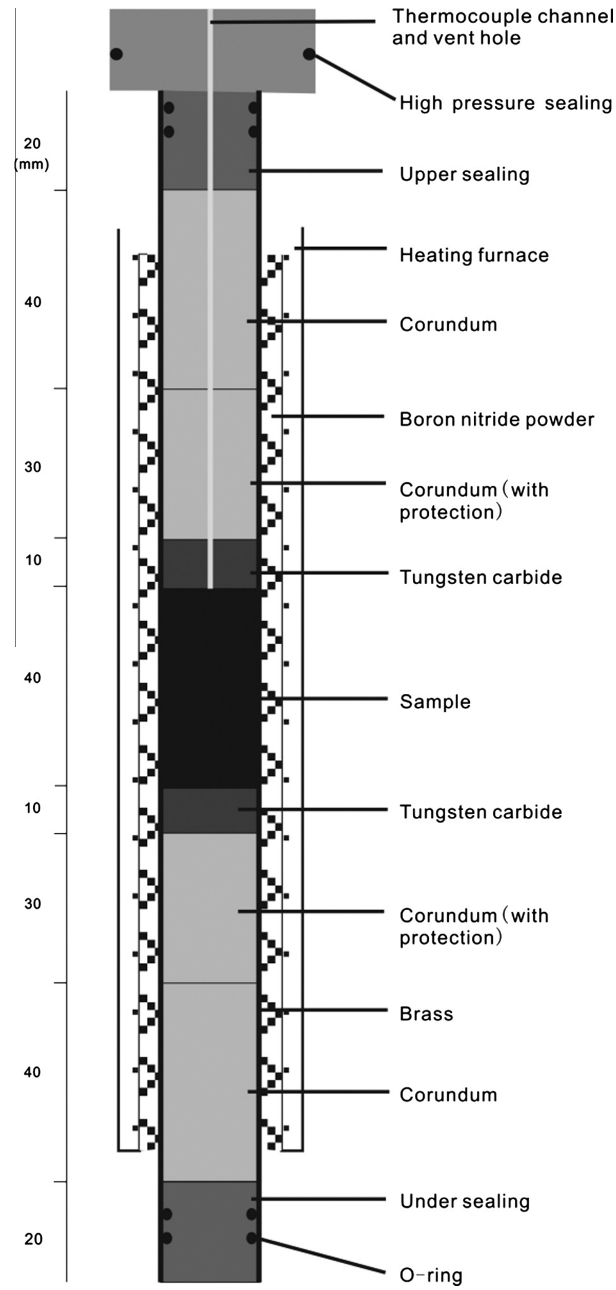

Fig. 2. The holding device for the sample.