

Response of Macromolecular Structure to Deformation in Tectonically Deformed Coal

LI Xiaoshi¹, JU Yiwen¹, HOU Quanlin^{1,*} and FAN Junjia²

¹ Key Laboratory of Computational Geodynamics, Chinese Academy of Sciences; College of Earth Science, University of Chinese Academy of Sciences, Beijing 100049, China

² PetroChina Research Institute of Petroleum Exploration and Development, Key Laboratory of Basin Structure and Petroleum Accumulation, Beijing 100083, China

Abstract: The structural evolution of tectonically deformed coals (TDC) with different deformational mechanisms and different deformational intensities are investigated in depth through X-ray diffraction (XRD) analysis on 31 samples of different metamorphic grades ($R_{o, \max}$: 0.7%–3.1%) collected from the Huaibei coalfield. The results indicated that there are different evolution characteristics between the ductile and brittle deformational coals with increasing of metamorphism and deformation. On the one hand, with the increase of metamorphism, the atomic plane spacing (d_{002}) is decreasing at step velocity, the stacking of the BSU layer (L_c) is increasing at first and then decreasing, but the extension of the BSU layer (L_a) and the ratio of L_a/L_c are decreasing initially and then increasing. On the other hand, for the brittle deformational coal, d_{002} is increasing initially and then decreasing, which causes an inversion of the variation of L_c and L_a under the lower-middle or higher-middle metamorphism grade when the deformational intensity was increasing. In contrast, in the ductile deformational coals, d_{002} decreased initially and then increased, and the value of L_c decreased with the increase of deformational intensity. But the value of L_a increased under the lower-middle metamorphism grade and increased at first and then decreased under the higher-middle metamorphism grade. We conclude that the degradation and polycondensation of TDC macromolecular structure can be obviously impacted during the ductile deformational process, because the increase and accumulation of unit dislocation perhaps transforms the stress into strain energy. Meanwhile, the brittle deformation can transform the stress into frictional heat energy, and promote the metamorphism and degradation as well. It can be concluded that deformation is more important than metamorphism to the differential evolution of the ductile and brittle deformational coals.

Key words: tectonically deformed coal, X-ray diffraction, deformational mechanism, deformational intensity, macromolecular structure

1 Introduction

Compared with other rocks, coal rocks are more sensitive to stress and strain, so their properties are easily affected by tectonic deformation. The tectonic deformation can not only change their primitive structure, but also change their macromolecular structure. Because macromolecular structure of tectonically deformed coals (TDC) is the important occurrence space for the coalbed methane (CBM), their change will have an influence on the occurrence state of CBM (Alexeev et al., 2004).

Obvious progresses on the analysis of coal structure and maceral compositions have been achieved during recent years by some scholars (Qu et al., 1980; Zhang and Dai, 1991; Cuesta et al., 1998; Yoshizawa et al., 2000, 2002; Jiang, 2001; Lu et al., 2001; Takagi et al., 2004; Zickler et al., 2006; Sonibare et al., 2010; Bernard et al., 2010; Cai et al., 2011; Shao et al., 2012). These studies indicated that, from lower to higher metamorphism coal, the chemical structure of different metamorphism coal showed a regular change. The aromatic rings are increasing and expanding, but the side chain of alicyclic compound and functional group is decreasing with the rise of metamorphic grade, and the main compound is polycondensation aromatic

* Corresponding author. E-mail: quhou@ucas.ac.cn

rings when it comes to anthracite (Wang and Pan, 1981; Levine and Davis, 1989; Qin, 1994; Khorasani et al., 1990). It is well-known that metamorphism in different degrees is a must for the formation of coal, while the deformation is not essential. For those coal rocks that experienced deformation, the deformation process and mechanism are various even when some of them were influenced by the tectonic deformation. Remarkable differences of macromolecular structure changes are shown between the TDC and the primary structure coal, which can be reflected from XRD analysis (Wang and Zhang, 1997; Jiang et al., 1998; Li et al., 2003; Ju et al., 2005a; Ju and Li, 2008). Furthermore, previous scholars have studied different aspects of coal structure. Levine et al. (1989) studied the relationship between tectonic deformation and coal optic character; Sonibare et al. (2010) summarized that the coals not only contain some crystalline carbon having turbostratic structure but also have a significant proportion of highly disordered amorphous carbon. And they compared the structural parameters, elemental carbon and volatile matter contents. Jiang and Cao discussed the influence of tectonic stress on coalification and presented the concept of stress degradation and stress polycondensation mechanisms (Jiang et al., 2001; Cao et al., 2007). Ju and Lin made a desk study on the changes of macromolecular structure under different deformations (Ju

et al., 2005a; Lin et al., 2009). Generally, the maximum of vitrinite reflectance ($R_{o, \max}$) can reflect the metamorphic grade, and the deformational intensity can be reflected by the relative anisotropy of reflectivity $((R_{o, \max} - R_{o, \min})/R_{o, \max})$, which is increasing when the deformational intensity increases (Chandra, 1965a, 1965b; Ghosh, 1970; Jones and Creaney, 1977; Davis, 1978; Ju et al., 2004a; Wu, 2010).

In the present study, we compared the XRD parameters of TDC with different deformation mechanisms and analyzed the different evolutions rules that change with the metamorphism ($R_{o, \max}$) and deformation $((R_{o, \max} - R_{o, \min})/R_{o, \max})$ in order to figure out the effect process and restriction mechanism of macromolecular structure under different deformations (brittle and ductile deformation).

2 Regional Geological Setting and Materials

As one part of the fold and thrust belt in the Mesozoic Dabie-Sulu collision orogen, the Xu-Huai area is located in the southeast of the North China Plate, and is adjacent to the Tanlu depth fault in the east and the Dabie orogen in the south. This area experienced multiperiod tectonic movements, and complex and unique fold fault systems were formed (Fig. 1). A series of shovel shape faults are distributing with a NS-NE strike, and the fold structures

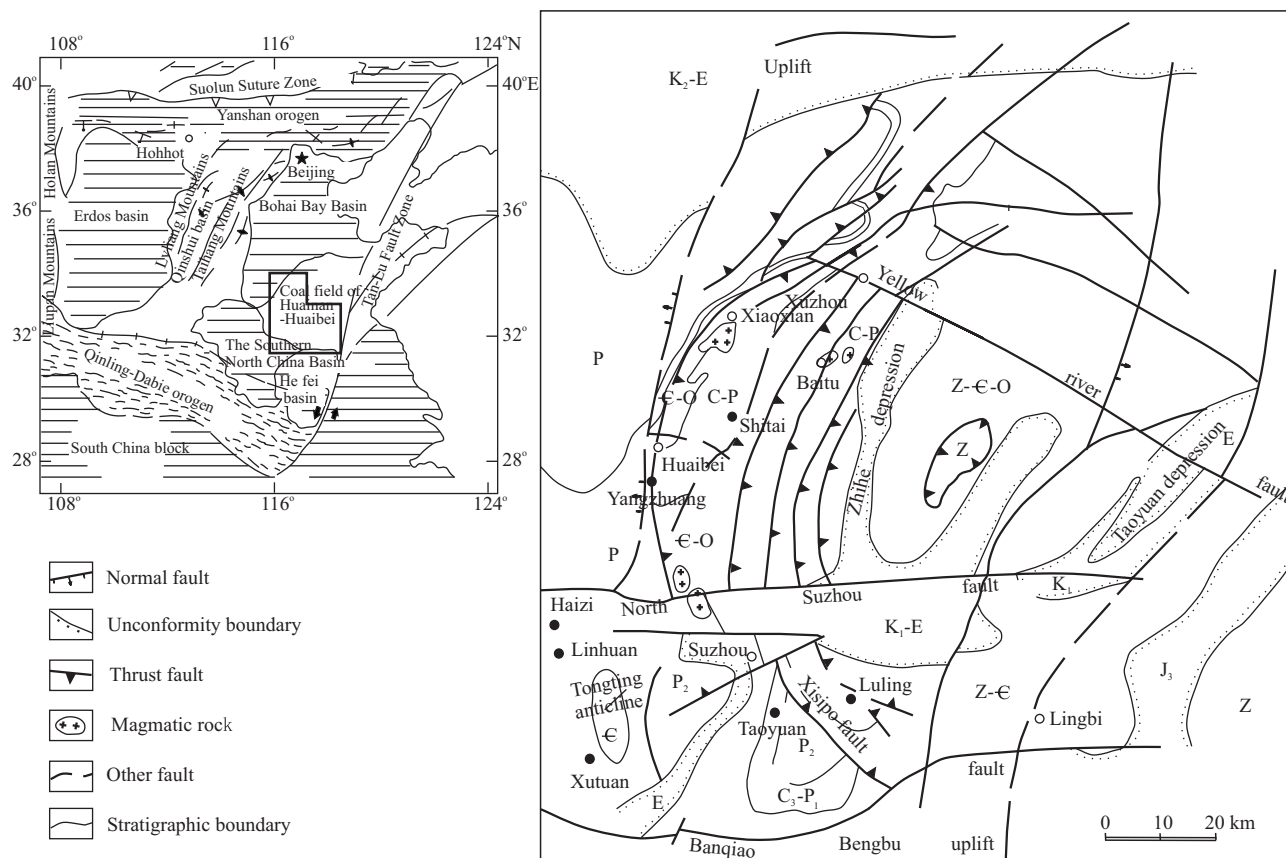


Fig. 1. The samples distribution plot (after Ju et al., 2005a).

are mainly with a NS–NNE axial direction. This tectonic association controlled the distribution of coal seams in the Huaibei coal field.

The samples were collected from the Permo-Carboniferous coal bed, which was strongly affected by the Mesozoic tectonic deformation. The coal seams are mainly reserved in the graben part especially in the syncline. The tectonic deformation can remarkably rebuild the coal seam as well as the inner structure of coal. Therefore, TDCs are widely developed in the strong tectonic deformation areas. The sampling places include the Yangzhuang and Shitai coal mines in the north of the Subei fault, and the Taoyuan, Luling, Linhuan, Xutuan and Haizi coal mines in the south.

Thirty-one TDC samples were performed on XRD tests in this paper. These samples were chosen based on their metamorphic grade ($0.7\% < R_{o, \max} < 3.1\%$) and deformational mechanism including brittle or ductile deformation. The types of these samples are based on the research of structure-genetic classification system by Hou and Ju (Hou et al., 1995a; Ju et al., 2004b). These samples are classified into three types: brittle, brittle-ductile and ductile deformation series. We chose two of them for this study: brittle and ductile deformation. Because the brittle-ductile deformation will complicate the affect reason of structure parameters, and will complicate the influence

mechanism of macromolecular structure.

3 Experimental Methods and Results

Before XRD testing, these samples were pretreated as follows. The first step was to demineralization, using HCl and HF to reduce the proportion of mineral matter in each sample until lowers than 2%. Then following the vitrinite centrifugation, the vitrinite was refined to 80%–90% using benzene and CCl_4 . These preliminary treatments can make sure samples have better TDC characters in XRD tests. In the mean time, the group maceral and vitrinite reflectance ($R_{o, \max}$) were tested as well.

The XRD analyses were performed on D/Max-RC X-diffraction spectrometer at the geological lab center in the China University of geosciences. The scan ranges from 2.5° to 135° , and in a continuous mode with a resolution of $2\theta=0.002^\circ$.

The spacing of aromatic layers (d_{002}), the stacking and extension of the basic structural unit (BSU) layer (L_c and L_a), aromatic layer number (N), aromatic ring number (n) and L_a/L_c can be achieved basing on the XRD spectrogram, by means of Bragg's and other equations (Wang and Pan, 1981; Ju et al., 2004b; Zhang et al., 2007) and the results in this research are listed in Table 1.

Table 1 X-ray diffraction (XRD) structural parameters of TDC samples

Series of deformation	Sample numbers	$R_{o, \max}$ (%)	$R_{o, \min}$ (%)	$^*\Delta R_o/R_{o, \max}$	d_{002} (nm)	L_c (nm)	L_a (nm)	N	L_a/L_c	n
Primary Structure coal	TY15	0.74	-	-	0.3825	0.8551	1.4109	2.24	1.65	29.9
	BJ10	0.89	-	-	0.3792	1.0164	1.6161	2.68	1.59	39.2
	ZXZ03	0.98	-	-	0.3745	1.0577	1.7073	2.82	1.61	42.9
Series of Brittle deformation	LHM06	0.98	0.83	0.22	0.3567	1.8005	4.2175	4.22	2.34	267.8
	HZM03	1.93	1.67	0.13	0.3477	3.8679	1.1279	8.40	0.29	19.2
	HZM04	2.08	1.82	0.13	0.3448	3.2743	1.9602	7.26	0.60	57.9
	SK04	1.00	0.91	0.09	0.3642	1.5270	2.8544	3.65	1.87	122.7
	TYM06	0.86	0.75	0.13	0.3633	1.7543	1.5294	4.09	0.87	35.2
	YZM12	1.69	1.31	0.22	0.3517	2.0249	1.2513	4.70	0.62	23.6
	YZM14	1.61	1.22	0.24	0.3472	2.5633	1.4015	5.81	0.55	29.6
	HZM02	1.93	1.67	0.13	0.3498	1.1948	2.0035	3.07	1.68	60.4
	LHM12	1.37	1.13	0.18	0.3520	2.1050	1.5596	4.86	0.74	36.6
	STM02	1.41	1.12	0.21	0.3570	1.9491	1.2337	4.51	0.63	22.9
	TYM04	0.95	0.8	0.16	0.3675	1.2480	1.3303	3.10	1.07	26.6
	LLM10	1.02	0.81	0.21	0.3660	1.3263	1.1646	3.25	0.88	20.4
	SK03	0.98	0.88	0.10	0.3542	1.7860	1.4467	4.21	0.81	31.5
	LLM01	1.16	0.9	0.22	0.3545	1.7711	1.5758	4.18	0.89	37.4
	SK08	1.09	0.94	0.14	0.3660	1.2126	1.3759	3.04	1.13	28.5
Series of ductile deformation	LHM04	1.40	1.18	0.16	0.3599	1.6463	1.2470	3.90	0.76	23.4
	LHM09	1.39	1.12	0.19	0.3621	1.6084	1.4455	3.82	0.90	31.5
	LLM04	0.83	0.6	0.22	0.3907	0.9281	1.6361	2.42	1.76	40.3
	STM01	1.54	1.26	0.18	0.3562	1.7560	1.7773	4.14	1.01	47.6
	XTM02	1.17	0.99	0.15	0.3590	1.6213	1.3653	3.86	0.84	28.1
	HZM10	2.62	2.02	0.23	0.3542	2.1468	1.6426	4.92	0.77	40.6
	LHM02	1.38	1.08	0.22	0.3499	2.1701	1.1011	5.00	0.51	18.3
	LHM03	1.58	1.18	0.25	0.3579	1.8156	1.2742	4.25	0.70	24.4
	LLM05	0.86	0.60	0.30	0.3701	1.1558	2.3762	2.91	2.06	85.0
	STM05	1.66	1.12	0.27	0.3520	2.2146	1.2776	5.07	0.58	24.6
	XTM08	1.92	1.63	0.21	0.3517	2.3623	1.9374	5.37	0.82	56.5

$^*\Delta R_o = R_{o, \max} - R_{o, \min}$; The data of primary structure coal comes from Ju, et al., 2005a.

4 Analysis and Discussion

4.1 XRD spectrum comparison

The XRD spectrum comparison showed that, with the increase of metamorphic grade, the diffraction peak of 002 (band at 12–13°) becomes higher and sharper, and the peak shape gradually tends more to symmetry. Meanwhile, the peak of 001 (band at 41–46°) is obvious.

There are different evolution ways that showed in XRD spectrum with the increasing of deformational intensity. The peak of 002 is lower, the full width half maximum is broad, the symmetry of the peak is reduced, and the peak of 001 gradually disappears (Figs. 2, 3). The influence of metamorphism and deformation on TDC macromolecular structure is completely different according to the above analysis.

4.2 Evolution characteristics of XRD parameters

4.2.1 Spacing of aromatic layers (d_{002})

Research on the relationship between d_{002} and metamorphism ($R_{o, \max}$) has made some progress. Qin (1994) found that the value of d_{002} is reducing, and has some stage characteristics with the rise of metamorphic grade. The reduction rate of d_{002} is slower when it reaches the anthracite grade, and gradually turns to 0.335 nm in the graphite crystal lattice of primary structure coal (Jiang et al., 1998; Luo and Li, 2004; Ju et al., 2005a). With the increasing of metamorphic grade, the evolutionary trend of d_{002} , both brittle deformational coal and ductile deformational coal, was basically identical with the one of primary structure coal (Fig. 4a).

However, there has been little research about the relationship between d_{002} and deformation ($\Delta R_o/R_{o, \max}$) of TDC. In fact, the d_{002} of different types of TDC is not only related with deformation, but also shows a different evolution trend (Fig. 4b). We divided the samples into lower-middle and higher-middle metamorphism grade in order to eliminate the influence of metamorphism. In the lower-middle metamorphism grade, d_{002} is increasing at first and then decreasing in brittle deformational coal, but changed in the opposite way resulting in bigger change ranges in the ductile deformational coal with increases of deformational intensity (Fig. 4b). In the higher-middle metamorphism grade, the change of d_{002} is the same as in the lower-middle metamorphism grade, but there were bigger change ranges in the brittle deformational coal. The influence of different evolutions of brittle and ductile deformational coal by deformation strength is obviously higher than the metamorphic grade (lower-middle or higher-middle metamorphism grade). So the main reason for the induced d_{002} difference in the evolution of TDC (brittle and ductile deformation) is not metamorphism but

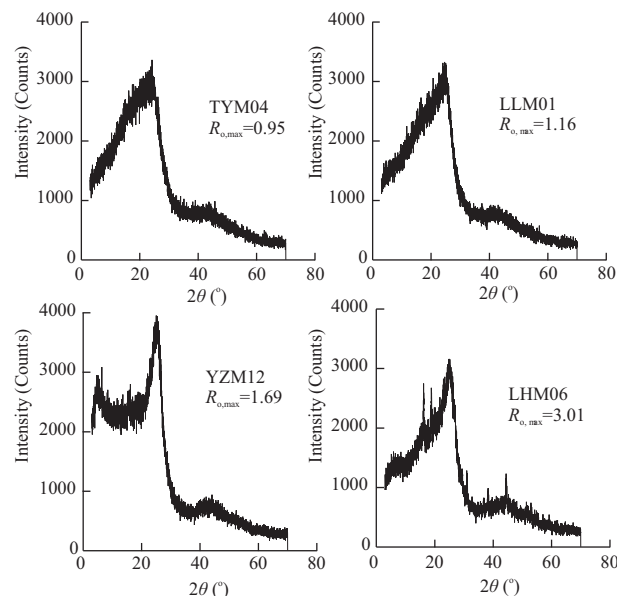


Fig. 2. X-ray diffraction (XRD) spectrum of different metamorphic grade.

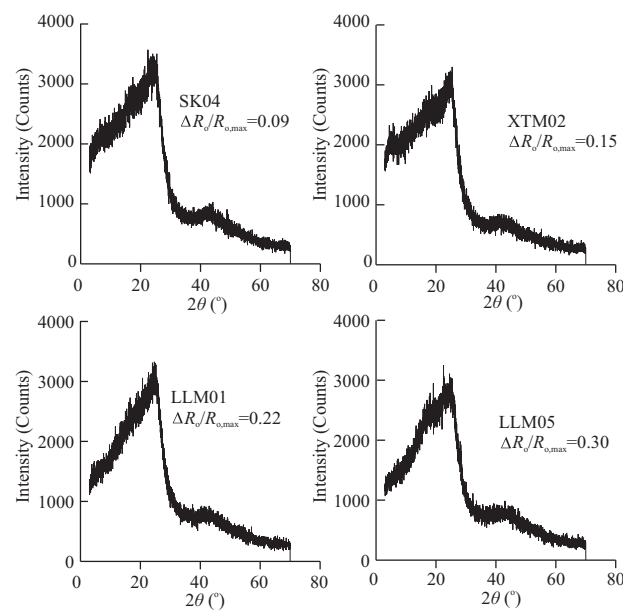


Fig. 3. X-ray diffraction (XRD) spectrum of different deformational intensity.

$$\Delta R_o = R_{o, \max} - R_{o, \min}$$

deformation.

4.2.2 The stacking of the BSU layer (L_c) and aromatic layer number (N)

The stacking of the BSU layer (L_c) to a certain extent can show the ordering degree of coal structure. Qin et al. studied the high metamorphic coal and proposed that the evolution of L_c is not a linear increase but a process of increase → decrease → increase and the same as the L_c evolution (Qin, 1994; Jiang et al., 1998). Ju et al. thought

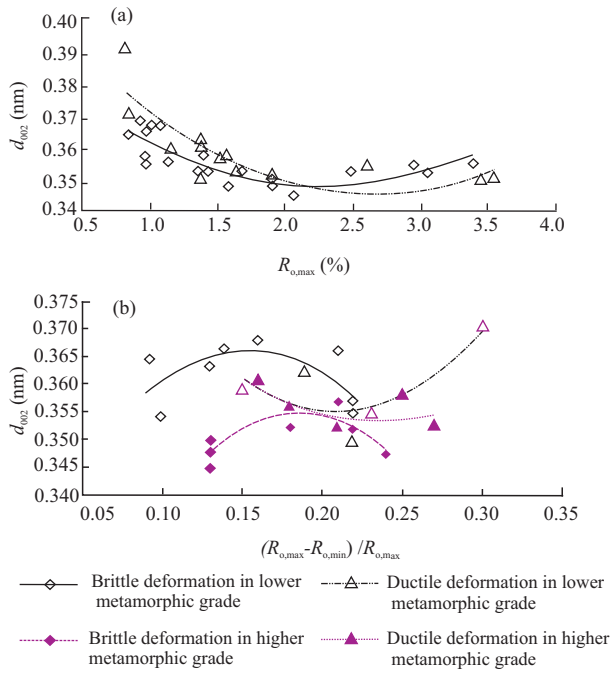


Fig. 4. Relationship between d_{002} and (a) metamorphic grade; (b) deformational intensity (partial data of low metamorphic grade are come from Ju et al., 2005a).

that the general L_c evolution of TDC is increasing and has step volatility changes in different stages (Ju et al., 2005a).

With the rise of metamorphic grade, the evolution of L_c and N in primary structure coal is increasing when the $R_{o,max}$ is between 2.5% and 3.5% (Jiang et al., 1998; Li et al., 2003; Ju et al., 2005a), which is inversed in TDC (Figs. 5a, 5b). The evolution trend of L_c and N are basically the same with the increase of metamorphic grade. It proved that the metamorphism has little effect on L_c and N of different deformational mechanism coals. With the increase of deformational intensity, L_c and N are decreasing at first and then increasing a little in brittle deformational coal, which is decreasing obviously in the ductile deformational coal under lower-middle metamorphism grade. But in the higher-middle metamorphism grade, L_c and N are decreasing at first and then increasing obviously in brittle deformational coal and changed to the opposite way in ductile deformational coal (Figs. 5c, 5d).

The evolution processes of d_{002} and L_c is opposite (Figs. 4b, 5c). With the increase of deformational intensity, d_{002} is increasing when L_c is decreasing to supplement the reduced value of L_c and keep the stability of the macromolecular structure. There is a complementary relationship between d_{002} and L_c . The change of d_{002} obviously plays as a buffer action and this perhaps prevents the sharp change of the macromolecular structure, which can breach its structure stability.

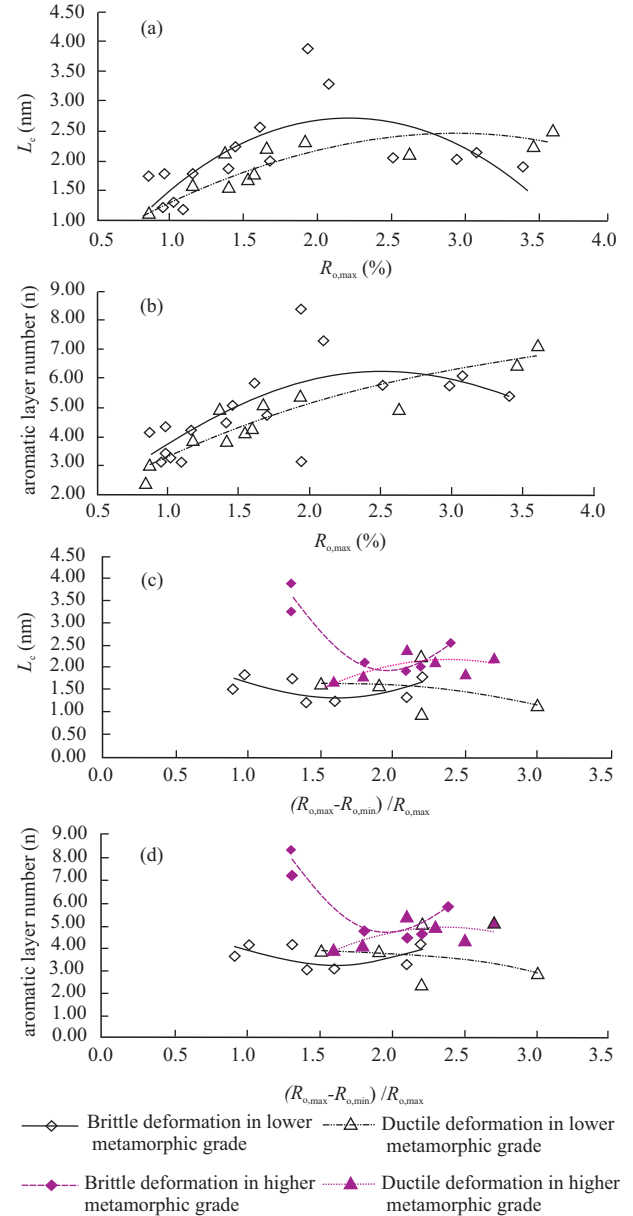


Fig. 5. Relationship between (a) metamorphic grade and L_c ; (b) metamorphic grade and aromatic layer number; (c) deformational intensity and L_c ; and (d) deformational intensity and aromatic layer number.

4.2.3 The extension of the BSU layer (L_a), aromatic ring number (n) and L_a/L_c

With the increase of metamorphic grade, the evolution of L_a and n are decreasing at first and then increasing. The evolution of L_a/L_c is similar but the reduction is much bigger. The same evolution trend of these parameters proved again that the metamorphism has little effect on the physicochemical property of coals (Figs. 6a, 6b, 7a). With the increase of deformational intensity, L_a and n are decreasing at first and then increasing in brittle deformational coal under lower-middle metamorphism grade, but the L_a/L_c is decreasing all the time, while the L_a ,

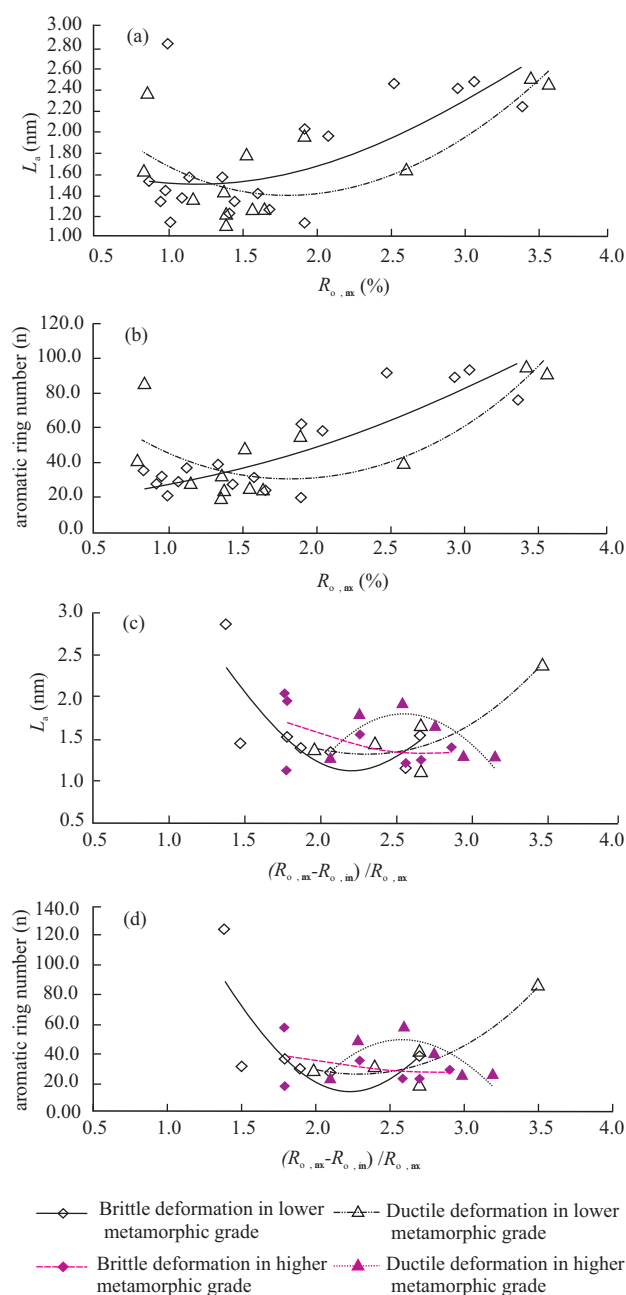


Fig. 6. Relationship between (a) metamorphic grade and L_a ; (b) metamorphic grade and aromatic ring number; (c) deformational intensity and L_a ; and (d) deformational intensity and aromatic ring number.

n and L_a/L_c is increasing in ductile deformational coal (Figs. 6c, 6d, 7b). But in the higher-middle metamorphism grade, L_a and n are decreasing at first and then increasing slightly in brittle deformational coal, but the L_a/L_c changed the opposite way with the increase of deformational intensity. While the L_a , n and L_a/L_c are increasing at first and then decreasing in ductile deformational coal (Figs. 6c, 6d, 7b).

Thus, the deformational intensity is the main reason that induced the different evolution of brittle and ductile

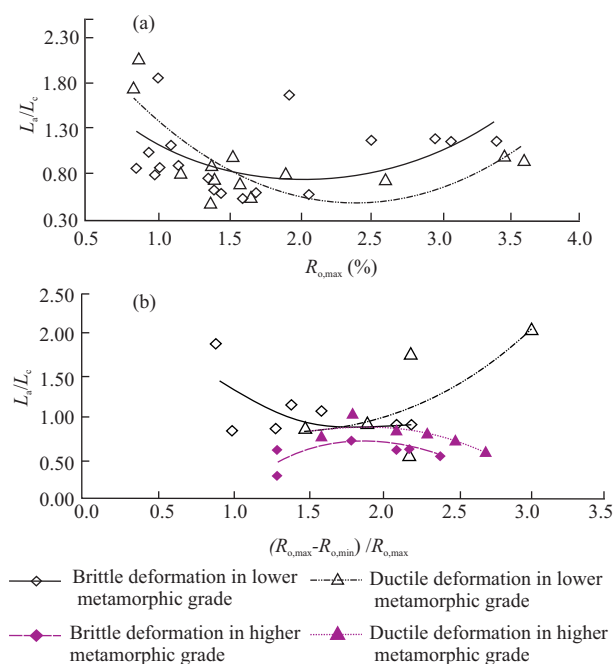


Fig. 7. Relationship between L_a/L_c and (a) metamorphic grade; (b) deformational intensity.

deformational coals. We will mainly discuss the process and mechanism of macromolecular structure, which affected by deformation in the following paragraphs.

4.3 Response of macromolecular structure to deformation process

In previous studies, scholars viewed that the evolution of L_c and L_a are increasing with the increase of metamorphic grade, which means that the polycondensation reaction of aromatic rings happened both in directions of stacking and extension of the BSU layer (Jiang et al., 1998; Luo and Li, 2004; Ju et al., 2005a; Cao et al., 2002). However, our research indicates that the evolution process of L_c is reverse to L_a . In the lower metamorphic grade, L_c is increasing and L_a is decreasing. This means that the degradation happened in the direction of L_a and polycondensation in the direction L_c . In the higher metamorphic grade, L_c is decreasing and L_a is increasing. This means that the degradation happened in the direction of L_c and polycondensation in the direction L_a . We also found that the metamorphic grade and deformational intensity have different influences on brittle and ductile deformational coals (Fig. 8). So why are the structure evolution processes of TDC and the primary structure of coal so different? We thought that the main reason is the deformational intensity and mechanism.

Both metamorphic grade and deformational intensity have influence on brittle deformational coals. The brittle deformation is closely connected with metamorphism. Brittle deformation can transform the stress into frictional

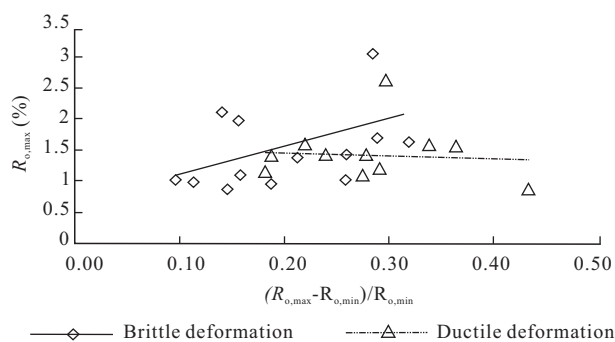


Fig. 8. Relationship between metamorphic and deformation in different deformation mechanism coals.

heat energy and promotes the metamorphism and degradation. However, the ductile deformation is mainly affected by deformational intensity. Because the ductile deformation can transform the stress into strain energy by increase and accumulation of unit dislocation of molecular structure (Hou and Zhong, 1993; Hou et al., 1995; Ju et al., 2004a). So it can have an obvious influence on deformation and polycondensation. Ju et al. studied the TDC using the ^{13}C NMR spectra and found that with the increase of deformational intensity, as carbon aromaticity (f_a) was raised further, carbon aliphaticity (f_{ai}) reduced obviously no matter what deformation mechanism it was (Ju et al., 2005b). This indicated, in the higher deformational intensity grade, the main action of macromolecular structure is stress polycondensation. However, the process is quite different. This will give us a new way to explain the reason that caused the different evolution of macromolecular structure between TDC and the primary structure coal.

In brittle deformational coals, under the lower-middle metamorphism and lower deformational intensity stage, the brittle deformation transforms the stress into frictional heat energy and promotes the metamorphism and degradation. The aliphatic functional groups, alkane branched chains and a fraction of aromatic rings in the direction of L_c and L_a are broken off by deformation and result in the reducing of L_c , L_a , N and n . Compared with the functional groups and branched chains between the aromatic rings in the direction of L_c , these small molecules that are linked on the edge of aromatic rings in the direction of L_a are much easier to break off. The cracking rate of functional groups and branched chains in the direction of L_a is faster and the cracking numbers are much greater. This caused the value of L_a to decrease faster and the value of L_a/L_c to also decrease. The aromatic rings are not combined by the dropped small molecules because of the rapid strain rate under the lower deformational intensity stage. With the increase of deformational intensity, these dropped small molecules are

randomly splice in the direction of L_c and L_a or transform into aromatic rings under the polycondensation. The splice speed of the dropped small molecules in L_c is increasing faster than L_a . This results in the L_c and L_a increasing, and the L_a/L_c decreasing.

But in the higher-middle metamorphism and lower deformational intensity stage, the small molecules in the direction of L_c start to break off because there are some small molecules that are linked on the edge of the aromatic rings in the direction of L_a left. So the cracking rate of aliphatic functional groups and alkane branched chains in the direction of L_c is faster and the cracking numbers are much greater. This caused the value of L_c to decrease faster and the value of L_a/L_c to increase. However, with the increase of deformational intensity, the dropped small molecules are splice in the direction of L_c or transform into aromatic rings, resulting in the value of L_c increasing and the value of L_a/L_c decreasing.

To sum up, for brittle deformational coal, the main action is stress degradation in the macromolecular structure of TDC under a lower deformational intensity stage, and this action is more obvious in the direction of L_a . But in the higher deformational intensity stage, the main action is change due to the stress polycondensation, and it is obvious in the direction of L_c .

For the ductile deformational coal, in the lower-middle metamorphism and lower deformational intensity stage, the change of L_c and L_a is not obvious because of the increase and accumulation of unit dislocation in molecular structure being slow. But with the increase of deformational intensity, both the degradation and polycondensation may occur in this stage. The unit dislocation of molecular structure is increasing and accumulating, which generates the unit dislocation that appears in the direction of L_a . The aliphatic functional groups and alkane branched chains in the direction of L_c start to break off and are splice in the direction of L_a or transform into aromatic rings. This results in the values of L_c decrease, L_a and L_a/L_c increasing.

In the higher-middle metamorphism and lower deformational intensity stage, the unit dislocation in molecular structure is increasing and accumulating to a certain amount, which generates the unit dislocation that appears in the direction of L_a and L_c in various degrees. The values of L_c and L_a are increasing. And L_a increased more because there were already unit dislocations in the direction of L_a . With the increase of deformational intensity, the dropped small molecules will form aromatic rings in this stage because the strain rate during ductile deformation is slowed. The unit dislocation in L_c and L_a makes the stability of molecular structure decreased, and leads to the aliphatic functional groups, alkane branched

chains and a fraction of aromatic rings in the direction of L_c and L_a breaking off by degradation. These dropped small molecules are replenished and embedded into the dislocation interspaces, and/or residual aromatic rings are formed into aromatic structure in the direction of L_a . When there is no place left in the direction of L_a to these dropped small molecules, they turn to the direction of L_c , then the value of L_c increases, L_a and L_a/L_c decreases.

Therefore, for ductile deformational coal, the stress degradation and stress polycondensation are both main actions in the macromolecular structure of TDC under the lower deformational intensity stage. The unit dislocation appears in the direction of L_a and L_c in various degrees. While in the higher deformational intensity stage, the main action is the stress polycondensation. The dropped small molecules are replenished and embed into the dislocation interspaces and/or residual aromatic rings are formed into aromatic structure in the direction of L_c and L_a .

5 Conclusions

(1) The deformational intensity and metamorphism have different influences on the TDC macromolecular structure. With the increase of deformational intensity, the macromolecular structure of the ductile and brittle deformational coals has various evolution ways. The deformational intensity has relatively more effect on the physicochemical property than metamorphism.

(2) The evolution processes of d_{002} and L_c are reversed under the deformational intensity. The change of d_{002} plays a buffer action, and this perhaps prevents the sharp change of the macromolecular structure, which can breach its structure stability.

(3) The brittle deformation transforms the stress into frictional heat energy, which not only plays a catalytic agent for the metamorphism process, but also promotes the degradation of macromolecular structure. For the brittle deformational coal, in both lower-middle and higher-middle metamorphism grade, the main action in the evolution process of macromolecular structure is stress degradation, which resulted in reducing of the L_c and L_a in lower deformational intensity stage. In this stage, the aromatic ring is not combined by the dropped small molecules because of the rapid strain rate. With the increase of deformational intensity, the main action is changing to the stress polycondensation, which induces the increasing L_c and L_a . The metamorphism is less important to the differential evolution than brittle deformation.

(4) In the lower-middle metamorphism and lower ductile deformational intensity stage, the change of L_c and L_a is not obvious. The degradation and polycondensation

are occurring with the increase of deformational intensity. Small unit dislocations appear in the direction of L_a . The aliphatic functional groups and alkane branched chains in the direction of L_c start to break off and are splice or transform into aromatic rings in the direction of L_a . In the higher-middle metamorphism and lower ductile deformational intensity stage, the unit dislocation appears in the direction of L_a and L_c in various degrees. However, in the higher deformational intensity stage, the dropped small molecules, which come from L_c and L_a are replenished, embed into the dislocation interspaces and/or residual aromatic rings are formed into aromatic structure in the direction of L_a first and then in L_c . Both the degradation and polycondensation are occurring in the lower ductile deformational intensity stage, and in the higher deformational intensity stage, the main action is the stress polycondensation.

Acknowledgements

This work was supported by the National Natural Science Foundation of China (Grant Nos. 41030422, 40972131, 40772135 and 41202120), the National Basic Research Program of China (Grant Nos. 2009CB219601 and 2006CB202201) and the China Postdoctoral Science Foundation Funded Project (2012M510590).

Manuscript received Nov. 11, 2011

accepted Mar. 16, 2012

edited by Liu Lian

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