STRUCTURAL AND CHEMICAL ALTERATIONS OF MIDDLE RANK COAL AT CARBONIZATION

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Introduction

Earlier was shown that the both heating temperature is the main factor that could influent at coal decomposition and yield thermodecomposition products which will be dependence from structure parent coal and process conditions [1,2], X-ray diffraction is a method that lets to find the alteration of middle rank coal at carbonization. Its method also could estimate a behavior the coal at carbonization.

Experimental

The Donbas deposit of middle rank coal was taken as object of investigation. Coal contained (%); $C^{daf} = 87,2$; $D^{daf} = 5,5$; $O+N^{daf}) = 2,3$; $A^{c} = 18,0$; $S^{d}_{t} = 5,0$; $V^{daf} = 33,0$. Coal carbonization (fraction less 0,5 mm) was carried out within temperature region 350-900°C in autoclave under vacuum, heating rate 10°C/min, time was 1 hour. The parent coal structure and carbonized residues with the both methods X-ray diffraction and i.r.-spectroscopy have been studied.

Results and Discussion

X-ray diffraction profiles studied coal is presented in Fig 1. It is shown that the most reorganization of structure coal taking place at temperature 3500°C. It is proposed that the both destroying large ordering globular structures of coal and following passes in the plastic state takes place. Also alterations in mineral part of coal was being observed. Reflections at 21 and 270°C (as quartz) were decreased. Apparently at 350°C redistribution of minerals within coal takes place. At rising carbonization temperature up to 500°C and more the increasing of reflections at 21 and 270°C take place. Also the reflections at 44, 50, 53 and 600°C are being appeared. It could propose that the formation of highly temperature aluminosilicates contained metals of K, Ca, Fe are being taken place.

Calculating of h/l_{002} parameter (a degree of interlayer ordering of crystallite) in carbonization temperature region (up to 900°C) confirms that the coal has a several stages of structural reorganization. In first stage a value of h/l_{002} parameter was decreased to the 0,47. It is proposed that destroying of the large ordering globular fragments in this stage takes place with a following coal passcd into the plastic state. In second stage (350-500°C) a value of h/l_{002} parameter was being increased and its maximun was 1,95. Earlier thermogravimetric method having been also shown that it is temperature region characterized the both highly temperature rate of coal decomposition and its conversion can achieve up to 35.0%.

It is being proposed that the tempeature region characterizing as a highly intensive decomposition reactions as a beginning the condensation reactions. In third stage coal carbonization (500-700°C) a value of h/l_{002} parameter was not being increased. Its parameter has a tendency to decreasing up to 1,5. Apparently, the reorganization of packing crystallite was changing itself trending from vertical upon horizontal level. In fourth stage (700-900°C) a value of h/l_{002} parameter was being increased up to 1,85. Apparently, it could be a result changed trending the reorganization of packing crystallite itself from horizontal to vertical level. It is also can be resulted structural changes within carbonized residue (for example, Lc, La, n parameters), Table 2.

It is shown (Table 1) that the changed trending the value of Lc, La parameters within temperature region 0-500°C is the same as for the curved was being illustrated at Fig.2. Decreasing of Lc parameter (a height of packing) with a together increasing La parameter (an average diameter of layer) could propose that the aromatic fragments condensed in the temperature region 500-700°C. Results Table 2 confirmed that the reorganization of packing crystallite at temperature above 500°C have two pathways: trending in vertical level when addition a new layers (n) in packing (Lc) takes place and a further changing itself trending from vertical level to horizontal level through condensed large aromatic fragments. IR-spectroscopy was shown that the pyrolysis liquid products have the adsorption bands at 1700 cm^{-1} and 1200-l150 cm^{-1} (ether bridges and phenol hydroxyl) pointing that the compound as dioxibenzene are these structural fragments could be closed to furan ring. Apparently structural changes within carbonized residue above 700°C and more can estimate as Lc/La ratio.

IR-spectrosoopy data carbonizated of middle coal are presented in Table 2. It is shown that the changes *E* adsorption bands at rising temperature carbonization take place. The most changing *E* adsorption bands carbonized residue i.r.-spetroscopy take place at 350°C. IR-spectroscopy data well correlated widt the X-ray diffraction data.

Conclusion

The results of X-ray diffraction and i.r -spectroscopy was shown that the middle rank coal at carbonization passes several stages of structural reorganization. Reorganization of packing crystallite up to 500°C trending to the vertical level determined as a changing a value of h/l_{002} parameter. Above 500°C the reorganization of packjng crystallite changes itself trending to horizontal level. One main parameter that could characterize its stage is a Le/La ratio.

References

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2. Shevkoplyas VN, Saranchuk VI. The impregnation effect on low and middle rank coals structural reorganization and their behavior dyring pyrolysis. Fuel 2000;79(4):557-565.

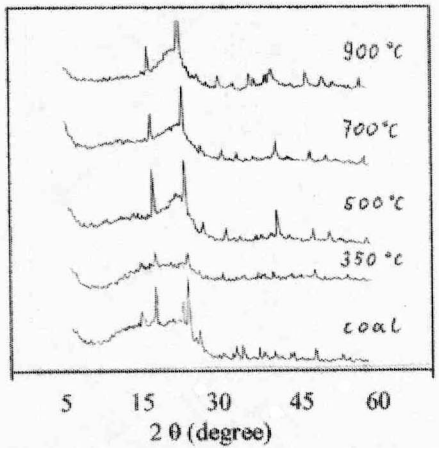

Figure 1 X-ray diffraction profiles of middle rank coal carbonized at various temperature

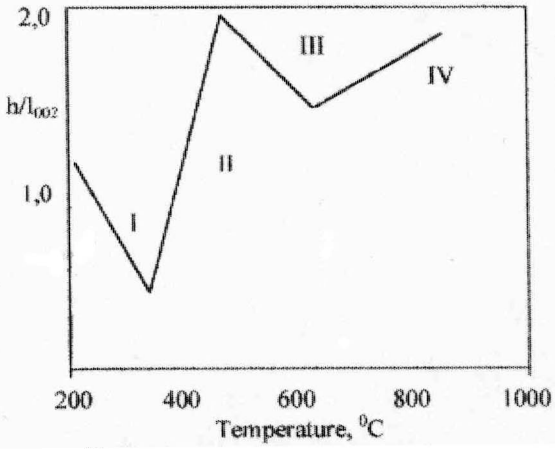

Figure 2 Alteration h/l_{002} parameter from carbonization temperature

Table 1 Changing X-ray parameters coal at carbonization

T °C	d_{002} (nm)	Lc (nm)	La (nm)	Lc/La	N
-	0,356	3,1	4,0	0,79	9,8
350	0,356	2,5	2,9	0,86	8,1
500	0,347	3,9	5,2	0,75	12,2
700	0,347	3,5	5,2	0,69	11,2
900	0,342	4,1	6,3	0,65	12,9

Table 2 Optical density *(E)* adsorption bands i.r.-spectra of coal at carbonization

T °C	3450	2950-2850	1600	1500	1450-1380	1300	1150-1050	870-750
-	0,23	0,12	0,16	0,10	0,13	0,13	0,14	0,07
350	0,27	0,15	0,26	0,12	0,20	0,20	0,25	0,09
500	0,13	0,07	0,14	0,13	0,22	0,17	0,20	0,10
700	0,19	0,04	0,13	0,14	0,18	0,18	0,29	0,10
900	0,26	-	0,16	0,15	0,16	0,21	0,33	0,13