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Relationship between coal ash composition and ash fusion temperatures

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HIGHLIGHTS

- This study is based on a five-component SiO_2–Al_2O_3–CaO–Fe_2O_3–K_2O system.
- This study uses a combination of XRD and SEM techniques.
- The effects of CaO, Fe_2O_3, K_2O and silica-to-alumina ratio on AFTs are studied.
- Conclusions found from synthetic ashes are applicable to real coal ashes.

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ABSTRACT

Coal ash fusion characterization and the ash fusion temperatures (AFTs) are important parameters for coal industry. Previous research has proved that the AFTs are correlated with the chemical composition of coal ash samples. In this paper, a five-component SiO_2–Al_2O_3–CaO–Fe_2O_3–K_2O system is set. The AFTs of 34 synthetic ashes were measured in a carbon atmosphere, and the trends of the AFTs analyzed. Different from other studies, X-ray diffraction (XRD) and scanning electron microscope (SEM) were combined to explore the relationships between the measured AFTs and the mineral composition, morphology and microstructure of ash samples. Furthermore, the effect of the element valence state is also taken into account and X-ray photoelectron spectrometer (XPS) is used to analyze it firstly. The results show that the AFTs decrease with the increasing Fe_2O_3 content and silica-to-alumina (S/A) ratio. However, for the effect of CaO content, the AFTs reach a minimum value and then increase once again. Furthermore, the AFTs show no significant change as the K_2O content varies. At last, all the conclusions found from the synthetic samples are also applicable for the seventeen bituminous coal ashes collected locally and abroad.

1. Introduction

The coal ash fusion temperature (AFT) is an important parameter on coal ash fouling and slagging properties. It determines the behavior of coal ash in the processes of coal combustion, gasification, liquefaction and ash utilization [1–3]. It can cause slagging problems on combustion chamber and pipe surfaces and decline heat transfer efficiency [4,5]. It is said that the operating temperature should be above the fluid temperature (FT) [6]. Thus, it is quite necessary to study the AFTs for not only theoretically, but for practical application.

There have been a number of studies carried out to calculate or predict the AFTs [7–9]. Jak used the thermodynamic computer package FactSage to study the relationship between AFTs and equilibrium phase diagram to develop a new AFT prediction method [10]. Seggiani developed the partial least-squares regression method to predict the AFTs [11]. Yin developed a back propagation neural network model to predict coal AFTs [12]. Some researchers also related the AFTs to the coal ash composition [13–15]. Gray et al. imported a multiple and stepwise regression analysis to investigate the correlation between ash composition and their AFTs [16]. Song changed the content of the primary oxides to study the effect of coal ash composition on AFTs [17]. These methods could not obtain highly precise results or could only be used in a limited range of conditions because of the complex chemical and mineralogical composition of coal ashes [18].

Coal ash is a mixture of oxides, so the properties of coal ashes at high temperature might be similar with the synthetic ashes composed by primary oxides [19]. Beside, the chemical composition of the synthetic ashes can be easily controlled. In order to simplify the experimental procedure and set up a model for application guidance, we decided to carry out research using synthetic ashes. We assembled 34 synthetic ashes mixed with SiO_2, Al_2O_3, CaO, and Fe_2O_3 to study the effects of CaO, Fe_2O_3 and silica-to-alumina ratio on the AFTs respectively. Besides, in order to consider the problem more rigorously, we considered to add one oxide, which had a low content in ashes to the system. It was said that initial

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deformation temperature (IDT) was mainly related to substantial melting of minerals containing K_2O in these ashes [20], thus, K_2CO_3 were added to the mixtures.

2. Experimental section

2.1. Coal ash samples

Seventeen typical coal samples were collected locally and abroad in this work. All the coal samples were ashed in air according to Chinese standard GB/T 1574-1995. All these samples are analyzed using X-ray fluorescence (XRF). The chemical compositions were presented in Table 1. The compositions of collected coal samples are used to determine the formula of synthetic ash samples.

2.2. Synthetic ash samples

Thirty-four synthetic ash samples whose chemical composition were based on the seventeen collected coal ash samples were prepared using SiO_2, Al_2O_3, Fe_2O_3, CaO and K_2O. The individual content is presented in Table 2.

2.3. Ash fusion temperatures

The AFT test supplies four temperatures which describes the softening and melting behavior of ash when it is heated: initial deformation temperature (IDT), spherical temperature (ST), hemispherical temperature (HT), and fluid temperature (FT) [21]. In this work, the AFT test was carried out in a carbon atmosphere which could be defined as weak reducing atmosphere according to Chinese standard GB/T 219-1996. In order to achieve a carbon atmosphere, we filled the testing corundum boat with enough graphite powder and made the furnace inclosed to ensure that ash cones are in protection of carbon during the whole testing procedure [22]. The AFTs results are presented in Table 1. After reaching the FT, the coal cones were natural cooled at 10 K/min and collected for instrumental analysis.

2.4. Instrumental analysis

The mineral composition of ash samples was determined by X-ray diffraction (XRD-600, SHIMADZU, Japan). The XRD curves were analyzed by the computer software package MDI Jade 5.0. The morphology and microstructure of an individual ash particle was analyzed using scanning electron microscope (SSX-550, SHIMADZU, Japan). The element valence state in ash samples were identified using X-ray photoelectron spectrometer (PHI5000 VersaProbe, ULVAC-PHI, Japan).

Table 2
Chemical composition of synthetic ashes.

No.	Composition of synthetic ashes (wt.%)					
	SiO_2	Al_2O_3	Fe_2O_3	CaO	K_2O	S/A
Ashes of different CaO content						
1	55.2	30.4	9.4	5.0	–	1.8
2	52.3	28.8	8.9	10.0	–	1.8
3	49.3	27.2	8.5	15.0	–	1.8
4	46.5	25.6	7.9	20.0	–	1.8
5	43.5	24.0	7.5	25.0	–	1.8
6	40.6	22.4	7.0	30.0	–	1.8
7	37.7	20.8	6.5	35.0	–	1.8
8	34.8	19.2	6.0	40.0	–	1.8
Ashes of different Fe_2O_3 content						
9	53.0	29.2	1.00	16.8	–	1.8
10	50.9	28.1	5.00	16.0	–	1.8
11	48.2	26.6	10.0	15.2	–	1.8
12	45.5	25.1	15.00	14.4	–	1.8
13	42.9	23.6	20.0	13.5	–	1.8
14	40.2	22.1	25.00	12.7	–	1.8
15	37.5	20.7	30.00	11.8	–	1.8
Ashes of different S/A ratios						
16	14.3	23.9	21.7	40.1	–	0.6
17	19.0	21.2	21.0	38.8	–	0.9
18	23.0	19.2	20.3	37.5	–	1.2
19	26.7	17.8	19.5	36.0	–	1.5
20	29.8	16.5	18.9	34.8	–	1.8
21	33.1	15.7	18.0	33.2	–	2.1
22	35.4	14.8	17.5	32.3	–	2.4
23	38.3	14.2	16.7	30.8	–	2.7
24	40.9	13.6	16.0	29.5	–	3.0
25	43.5	13.2	15.2	28.1	–	3.3
26	46.0	12.8	14.5	26.7	–	3.6
27	48.6	12.4	13.7	25.3	–	3.9
Ashes of different K_2O content						
28	48.9	27.0	8.4	15.5	0.2	1.8
29	48.7	26.9	8.3	15.4	0.5	1.8
30	48.5	26.7	8.3	15.3	0.8	1.8
31	48.3	26.6	8.3	15.2	1.1	1.8
32	48.1	26.5	8.2	15.2	1.4	1.8
33	47.8	26.4	8.2	15.1	1.7	1.8
34	47.6	26.3	8.1	15.0	2.0	1.8

Table 1
Chemical composition and AFTs of coal ash samples.

No.	Ash samples	Content of oxides (wt.%)											The AFTs (°C)			
		SiO_2	Al_2O_3	S/A	Fe_2O_3	CaO	MgO	K_2O	Na_2O	SO_3	TiO_2	P_2O_5	IDT	ST	HT	FT
1	Shanxi Datong	56.6	25.4	2.2	6.5	3.7	1.4	1.4	0.6	2.9	0.9	0.5	1239	1294	1308	1352
2	Heilongjiang Jixi	64.1	27.2	2.4	2.9	0.9	0.5	1.6	0.2	0.9	1.5	0.1	>1450	>1450	>1450	>1450
3	Shandong Xinwen	52.9	31.9	1.7	4.9	2.7	1.2	1.7	0.7	2.2	1.6	0.1	>1450	>1450	>1450	>1450
4	Anhui Huainan	50.8	36.0	1.4	6.1	1.9	0.6	1.3	0.3	1.4	1.3	0.2	>1450	>1450	>1450	>1450
5	Neimenggu lijiata	41.7	23.0	1.8	7.1	13.1	2.1	0.8	0.9	10.0	0.9	0.2	1141	1158	1165	1177
6	Liaoning Fuxin	52.7	33.5	1.6	5.9	1.8	1.1	0.7	0.3	1.4	1.5	1.0	>1450	>1450	>1450	>1450
7	Shanxi Huating	39.7	18.2	2.2	17.1	17.5	0.9	0.3	0.2	4.5	1.2	0.2	1160	1200	1220	1300
8	Shandong Zaozhuang	34.9	16.5	2.1	8.0	37.1	2.0	0.2	0.1	0.6	0.3	0.1	1180	1201	1208	1230
9	Shandong yanzhou	23.0	34.0	0.7	22.1	17.3	1.7	0.5	0.3	0.6	0.4	0.1	1155	1186	1198	1225
10	Shanxi gujiao	24.2	27.1	0.9	25.2	18.0	0.7	0.8	0.4	1.1	0.4	0.3	1220	1247	1253	1280
11	Sofia Bulgaria	32.0	11.3	2.8	10.6	27.7	2.8	1.1	0.2	3.2	0.7	0.2	1100	1120	1215	1225
12	Montana US	44.5	20.3	2.2	1.6	15.7	3.5	1.1	1.3	1.1	1.8	1.3	1125	1150	1200	1205
13	Miike Japan	47.7	20.8	2.3	10.2	9.7	1.5	1.0	2.1	1.7	1.2	0.1	1165	1180	1300	1320
14	New Hope Australia	62.5	30.0	2.1	2.6	0.9	0.4	0.5	0.9	0.6	1.2	0.1	>1450	>1450	>1450	>1450
15	Mafty Russia	60.6	21.9	2.8	5.1	5.0	1.9	1.1	0.5	0.7	0.7	0.5	1170	1190	1335	1360
16	Coal Mountain Canada	39.9	27.3	1.5	2.5	22.1	3.2	0.6	0.7	2.0	0.5	0.7	1200	1240	1380	1450
17	Donbass Ukraine	53.8	20.4	2.6	15.1	2.8	1.3	1.0	0.6	2.1	0.8	0.6	1150	1175	1355	1370

IDT, initial deformation temperature; ST, spherical temperature; HT, hemispherical temperature; FT, fluid temperature.