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Investigation on the structure evolution of pre and post explosion of coal dust using X-ray diffraction

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ABSTRACT

To reveal the effects of coal dust explosion on its crystal structures evolution, the micro structure of six different rank of coal dust and its explosion solid products had been studied using 20 L explosion sphere vessel and X-ray diffraction (XRD) analyzer. The correlations between structural parameters and explosion severity had been analyzed detailed. Results show that coal dusts with higher volatile matter contents (V_{daf}), lower vitrinite reflectance ($R_{o,max}$) and less ash contents (A_{ad}) show stronger explosion severity. The effects of vitrinite reflectance ($R_{o,max}$) on the explosion severity parameters present the same role as the influence of volatile matter contents (V_{daf}). Coal dusts with developed porous structure (S_{BET} and V_{BJH}) also present higher explosion reactivity. Interestingly, six selected coal samples present the strongest explosion severity at the same optimum explosion concentration (250 g/m^3). For the different rank raw coal, the difference of the shape and intensity of 002 peak varies greatly. With the decreasing of coal ranks, the 002 band tends to be blunt and the peak intensity is relatively short. Quantitative analysis show that the lattice parameters (L_a, L_c, and N_{avg}) of six coal samples are found to relatively increase with increasing vitrinite reflectance ($R_{o,max}$), whereas the d_{002} slightly decreases. The explosion treatments have significant effects on the ordering of coal aggregate structure. Compared with raw coal sample, the relative intensity of 002 bands at about 26° is reduced by the explosion treatments, which would increase the degree of graphitization of the explosion solid products. With the increasing of explosion pressure, the relative intensity of 002 peak would be gradually decreased. However, the shape of 002 peak for the explosion solid products tend to be more asymmetric and blunter than that at lower explosion conditions. Compared with the parent coals, the inter-layer spacing d_{002}, L_c and N_{avg} of all explosion products would be slightly reduced correspondingly. However, there is no clear rule for the evolution of L_a parameter. Moreover, calculated aromaticity (f_a) of the coals ranges from 0.2208 to 0.6883, which is linear positively increased with the coal maturity by vitrinite reflectance.

1. Introduction

Floating coal dusts are always produced during coal mining process in the underground mines [1,2]. In the coal mine and other coal processing or utilizing industries, there are always some safety problems, such as coal dust explosion accidents. Generally, surveys to the coal mine explosion accidents have shown that explosions are mostly accompanied by the participation of coal dust to some extent. Therefore, analyses on the coal dust and its explosion products play an important role in revealing the explosion mechanism and the causes of coal dust accidents [3]. All these data will be useful in the future forensic investigations of accidental dust explosions in coal mines.

Basically, coal dust explosion severity parameters are critical for the safety management and risk assessment in the coal mines. So, many researches had been focused on the investigations to key influencing factors on the coal dust explosion severity, such as dust concentration, limiting oxygen concentration, minimum ignition temperature, explosion severity parameters and explosion flame propagation behaviors. By experiments, Cashdollar [4], Going [5] and Bi [6] measured the minimum explosive dust concentrations (MEC) and limiting oxygen concentrations (LOC) of different coal dusts and pointed out that the particle physical properties, including coal particle size and the volatile contents, had an important effects on the explosion severity of coal dust. With 20-L spherical vessel and numerical simulation, Cao et al. [7]

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studied the correlations of explosion pressure and the explosion pressure rise rate with increased coal dust concentrations. In addition, with the help of in-situ diffuse reflection Fourier transform infrared spectrometry (FTIR), the functional group variation law before combustion of lignite coal dust had also been tested. Results demonstrated that the key functional groups influencing coal dust explosion were —CH_3, —CH_2— and —OH [8]. Using high speed video camera and thermal infrared imaging device, flame propagation velocity, the highest flame temperature and particle transient movement were tested. Result showed that both the flame propagation and the dust cloud expansion are first accelerated and then decelerated with the increasing of tube length. Moreover, the gas flow velocity was higher than the flame propagation velocity [9–11]. In addition, previous researches also showed that coal particle thermal characteristics and size distributions had great influence on flame structures and its propagating mechanisms during dust explosions [12]. Using two experimental tubes with different diameter and length, coal dust/air explosion experiments were performed by Bartknecht [13,14] and their results showed that small size coal dust produced great maximum explosion flame speed. Using the 20 L explosion sphere, Gao et al. [15] found that the lower explosion limit would be reduced with the decrease of particle size. For a given concentration, finer coal particles always caused higher explosion severity. Considering the effects of large particles, Man and Harris's [16] researches showed that coarse, medium, and pulverized Pittsburgh coal had similar P_{max} values, but the minimum explosion concentration (MEC) would be increasing with particle size increases. With the help of SEM and FTIR, Liu et al. [17,18] studied the microscopic structure of post-explosion samples and pointed out that there were significant differences of explosion properties between larger coal particles and smaller coal particles, including their microscopic characteristics of explosion products. Compared with smaller particles, the explosion of larger coal particles requires more rigorous conditions, such as higher dust concentration and larger ignition energy. Furthermore, using an approach combining high-speed photography and a band-pass filter, Gao et al. [19] reported that dust explosion flame propagation mechanisms would be changed from kinetics-controlled to devolatilization-controlled when decreasing the volatility of materials or increasing the size of particles. Especially, presences of flammable gases, such as methane, have significant accelerate to the coal dust combustion process and would cause substantial changes of flammability concentrations [20].

It is well known that coal is a complex porous carbonaceous material. Varieties of organic and inorganic matters involved in the formation of coal makes them highly heterogeneous, both in physical and chemical structure that vary with their degree of coalification. Generally, the nature and extent of the microstructural changes of coal upon oxidation conditions, the relation between microstructure and reactivity towards oxygen had been extensively addressed. Senneca et al. [21] reported that the major changes in morphology, structure and chemical composition of solid coal particles occur in the early instances of combustion/gasification processes. At this stage, particles would be broken into smaller fragments because of thermal stress and pressure generated by volatiles release. And, Senneca et al. [22] had also presented a model that goes beyond primary fragmentation and considers the effects of combustion of both char and volatiles within the pores on the fragmentation propensity of particles. Therefore, to some extent, the structural characterization of coal represents one of the most important information of their reactivity [23]. Using laser particle size analyzer, SEM, XRD and TGA, Zhao et al. [24] presented that presence of much more disordered crystalline structure and high porosity of carbonaceous materials in the particles were contributed to its reactivity. Using 20-L chamber and 1 m^3 chamber, Cashdollar et al. [25] collected the explosion products of high- and low-volatile bituminous coals and measured the incombustible content of these dust before and after the explosions. Their results showed that all coal dust that was suspended within the explosion flame produced significant amounts of coke and the post-explosion incombustible content was always as high as, or higher than the initial incombustible content. By analyzing the microstructures of first and secondary explosion residues, Hong et al. [26] reported that spatial distributions of C, Cl, and Si in the residues were uniform. However, the contents of Ca, Al, Si, Cl, and Fe increased, and the carbon content decreased as the reaction proceeded. Therefore, it can be deduced that the analysis of the microstructure of coal dust and its explosive products will provide some valuable information in further understanding the dust explosion reactivity, and even the inerting mechanism for coal dust explosion suppression.

Generally, coal consists of primary macromolecular structure and secondary aggregate structure, latter of which was derived from aromatic ring stacking, aliphatic side chain entanglement and hydrogen bonds bridges depending on the coal rank [27]. These components present as a series of graphene layers' state stacked in units of different number of layers (2–6) [28,29]. And, these structures and stacks vary with heat treatments. As a function of heat treated conversion process, micro structure of coals, including the interlayer spacing (d_{002}), crystallite sizes (L_c and L_a), the average number of aromatic layers per carbon crystallite (N_{avg}), the aliphatic chains and the aromaticity (f_a) of the coals, would be gradually evolved with the coal oxidation process [30–34]. Researches showed that after heat treatments, the stacking of the aromatic layers in the caking coal temporarily developed. Moreover, the average number of aromatic layers per carbon crystallite (N_{avg}) of the caking coals was larger than that of the non-caking coals. However, the release of volatile components partially disordered the stacked layers [35]. Furthermore, the heating rate required for the development of stacking structure in lower-rank coals was lower than that required for higher-rank coals [36]. It was supposed that these structures of coal play an important role in the conversion process.

Previous researches had shown that X-ray diffraction (XRD) used as a useful tool could provide much more qualitative and quantitative microstructure information about the oxidation properties of coal and other carbon materials [37,38]. And up to now, there is limited published result of investigation on the structure evolution during coal dust explosion process. In present research work, the micro structure of coal dust and its explosion solid residues had been studied and the correlations between structural parameters and explosion severity had been analyzed detailed.

2. Experimental section

2.1. Sample preparation and characterization

Six kinds of coal in different ranks are selected among Chinese typical coal fields. All samples are crushed and screened separately to pass through the 100 meshes sieve according to the experimental design. Proximate analyses of the six original coal samples (before drying process) were determined by an automatic proximate analyzer (5E-MAG6600) according to standard method of GB/T212-2001 [39] of China. And, the maximum vitrinite reflectance ($R_{o,max}$) of each coal samples was measured by microscopic spectrophotometer (ZEISS Imager M1m) according to the oiled refraction method of GB/T6948-2008 [40]. The results of proximate and vitrinite reflectance analysis of raw coal samples are listed in Table 1. Before the explosion tests, the screened coal samples are dried overnight at about 60 °C under nitrogen gas stream (2 ml/min) environment for moisture removal.