Study on multicomponent calcium ferrites formation by using XRD-Rietveld analysis

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ABSTRACT

Multicomponent calcium ferrites represented by Silico-ferrite of Calcium and Aluminum (SFCA: $Ca_2(Ca,Fe,Al)_6(Fe,Al,Si)_6O_{20}$) or SFCA-I($Ca_3(Ca,Fe)(Fe,Al)_{16}O_{28}$) are key mineral phases for exhibiting sinter ore properties. They are formed from calcium ferrite melt during the cooling process in the sintering reaction, which is a short period and non-equilibrium. Highly accurate quantification of SFCA and SFCA-I by conventional X-ray diffraction (XRD) analysis is difficult because their XRD patterns are similar and complicated. However, the determination precision could be improved by using Rietveld analysis, which is a pattern-fitting technique using the crystallographic parameters of existing phases and profile parameters.

The aim of this study is to research the formation conditions of multicomponent calcium ferrites and other phases by analysis of sintered tablet samples.

Mixtures of iron ore and reagent grade powder of $CaCO_3$, SiO_2, Al_2O_3 (CaO content of 0.91 mass%) were pressed into tablets (8mmφ*10mmH) and heated up to 1573 K with a heating rate of 200 K/min then cooled with a cooling rate of -66.7 K/min under air atmosphere. The compositional ratio of Al_2O_3 (0.33~2.33 mass%) and SiO_2 (2.36~4.36 mass%) was varied. Products were identified and quantified by powder XRD and Rietveld analysis

SFCA fraction in products were increased with increasing the concentration of Al_2O_3 (In case SiO_2 was a constant of 2.36 mass%). However, SFCA-I fraction was slightly decreased. The cause is considered to be that it approached the single-phases region of SFCA in the equilibrium diagram by adding aluminium oxide. Also, SFCA-I fraction was decreased with the addition of silicon oxide. It is considered that SFCA formed preferentially and SFCA-I hardly formed in the case of silicon oxide solved in calcium ferrite melt.

Consequently, it is considered that the gangue minerals melting (especially, silicon oxide) in the calcium ferrite melt is important for the control of SFCA or SFCA-I formation.

Keyword: Sinter, X-ray diffraction, Rietveld analysis, calcium ferrite, SFCA