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Deconvolution analysis of reflectance spectra of synthetic clinopyroxenes using the exchange Monte Carlo method

HONG, Peng[1*] ; MIYAMOTO, Hideaki[1] ; NAGATA, Kenji[2] ; SUGITA, Seiji[3] ; NIIHARA, Takafumi[1] ; JAMES, Dohm M.[1] ; HENMI, Ryodo[1] ; OKADA, Masato[2]

[1]Univ. Museum, Univ. of Tokyo, [2]Complexity Sci. & Eng., Univ. of Tokyo, [3]Earth & Planetary Sci., Univ. of Tokyo

Deconvolution analysis of reflectance spectra has been a useful method to infer mineral composition and crystal structure. Clinopyroxene (CPX) is one of the most important mineral groups due to both its rich abundance on solid bodies in the solar system and distinguished absorption features. The band centers of visible to near-infrared (Vis/NIR) spectra of CPX are known to vary due to total iron and calcium content. Klima et al. (2011) characterized the Vis/NIR spectra of synthetic CPX based on a modified Gaussian Model (MGM). The numerical algorithm of the widely used MGM (Sunshine et al., 2011), however, utilizes the steepest descent method, which has a local minima problem. With bad initial parameters, the steepest descent method converges into a local minimum, thus the analyzer needs to manually adjust initial parameters and calculate the model repeatedly to obtain the desired solution. In order to avoid the local minimum problem, we analyzed Vis/NIR spectra of CPX using Bayesian spectral deconvolution with the exchange Monte Carlo method (Nagata et al., 2012). This method is an improved algorithm of the Markov chain Monte Carlo method, aimed to both avoid local minima traps and remove the arbitrariness originated from initial parameters. We used the Vis/NIR spectra of CPX, measured by Klima et al. (2011) at 5 nm intervals over the wavelength range of 0.3-2.6 μm. We chose only sieved powder samples whose grain sizes are smaller than 45 μm with individual grains about 15-25 μm in size. We collected 31 CPX spectra with wide ranging Ca, Mg, Fe compositions (8-52%, 0-52% and 3-90%, respectively). We found that: (1) 1 μm band shifts regularly to longer wavelengths with an increase of Ca content; (2) 1 μm band shifts to shorter wavelengths with an increase of Fe content, although the variance is larger than that of orthopyroxene; (3) for Ca contents $<$30%, 2 μm band shifts to longer wavelength as a function of Ca, while for Ca contents $>$30%, the center of 2 μm band remains almost constant at ˜2.4 μm; and (4) the center of 2 μm band of augites (Ca $<$˜20%) does not depend on Fe content significantly, while the center of 2 μm band of pigeonites (Ca $>$˜20%) shifts to longer wavelengths as a function of Fe content. These results are consistent with Klima et al. (2011), suggesting that the exchange Monte Carlo method can yield the same results obtained by conventional MGM analysis. The successful application of the exchange Monte Carlo method to wide range of CPX would pave the way for further deconvolution analysis of reflectance spectra of mineral mixtures, such as olivine, orthopyroxene, and clinopyroxene.