Structural controls on surface hydroxyl reactivity in iron hydroxides

XIAOWEI SONG* AND JEAN-FRANÇOIS BOILY

Department of Chemistry, Umeå University, Sweden (*correspondence: xiaowei.song@chem.umu.se)

Mineral surfaces are populated with distinct types of hydroxyl groups displaying various catalytic roles with respect to gases, solvents and solutes. Knowledge of the types and distributions of hydroxyl groups on minerals with different surface structures is essential for gaining molecular-scale resolution of these processes.

This work provides Fourier transform infrared (FTIR) spectroscopic signatures of hydroxyl groups present on surfaces of FeOOH minerals, including lath- and rod-shaped lepidocrocite (γ), (nano) goethite (α) and akaganéite (β).

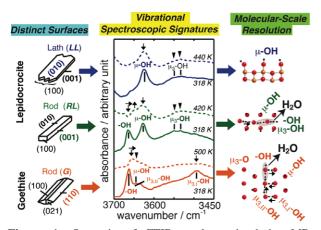


Figure 1: Synopsis of FTIR work, assisted by MD simulations, used to identify surface species and reactivity.

Our combined FTIR and molecular dynamics studies of these FeOOH surfaces enabled the extraction of unique spectroscopic signatures for distinct hydroxyl groups. Individual responses of these groups to variations in proton loadings and temperature provide experimental validation to previous theoretical accounts on their reactivity. These efforts now provide new possibilities for probing important gas-phase adsorption processes. They should moreover lay foundations for interfacial studies involving water.

La-Ce and Sm-Nd isotope geochemistry of felsic granulite in the Jirisan complex, Yeongnam Massif, Korea

YONG-SUN SONG¹, SEUNG-GU LEE^{2*}, YOSHIHIRO ASAHARA³ AND TSUYOSHI TANAKA³

¹Department of Earth Environmental Sciences, Pukyong National University, Pusan 608-737, Korea (yssong@pknu.ac.kr)

²Geological Research Division, Korea Institute of Geoscience and Mineral Resources, Daejeon 305-350, Korea (sgl@kigam.re.kr)

³Department of Earth and Environmental Sciences, Nagoya University, Nagoya 464-8601, Japan (asahara@eps.nagoya-u.ac.jp, tanaka@eps.nagoya-u.ac.jp)

REEs contain two long-lived decay systems, the ¹⁴⁷Sm-¹⁴³Nd and ¹³⁸La-¹³⁸Ce decay systems, which provide us with the information on ages and initial ratios that helps us understand their origin and history. Hence, the application of the La-Ce and Sm-Nd isotope systematics in petrogenetic studies has enabled an estimation of the light rare earth element (LREE) patterns in source materials of the rocks.

We report La-Ce and Sm-Nd isotopic data of highly evolved granites with the composition of major and rare earth element from the felsic granulite, which occurs at the Jirisan Complex in the Yeongnam Massif, Korea. Based on the Ce and Nd isotopic data, we also discuss the REE geochemistry of source material of the Jirisan felsic granulite. The felsic granulite shows three different types of chondrite-normalized REE pattern: one is a tetrad REE pattern of M-type with a large negative Eu anomaly, another is a W-type tetrad REE pattern, and the third is an REE pattern of crustal type showing an LREE-enriched and HREE-depleted pattern. U-Pb zircon and Rb-Sr whole rock ages are 1874 Ma and 1831±36 Ma (2σ) with initial 0.7028±0.0097, respectively. However, Sm-Nd isotopic system from these rocks shows error-chron ages from 1235 Ma to 1570 Ma suggesting that Sm-Nd isotopic system might have been disturbed by specific geochemical processes related to the formation of the tetrad REE patterns. Nevertheless, initial Ce-Nd isotopic values show that all three types were derived from the isotopically similar source materials. Our data also indicate that La-Ce and Sm-Nd isotopic system may be useful in understanding REE fractionation between rock and its source material.

Mineralogical Magazine

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