

MODELING OF INFRARED REFLECTANCE SPECTRA OF VOLATILE-RICH ASTEROIDS

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Introduction: The mineral assemblages on asteroids are useful to constrain the aqueous environments—the temperature (T), pressure (P), water to rock ratio (W/R), and bulk chemical composition—existed in them or in their parent bodies. The aqueous conditions reflect their formation and evolution processes: when, where, and how they have formed and evolved. The understanding of these small bodies would ultimately unveil the dynamic history of the solar system and the origins of volatile elements on terrestrial planets.

Near- to mid-infrared (IR) reflectance spectroscopy of asteroids contains the information of the surficial minerals in their characteristic absorption features, spectral slopes, and overall brightness or darkness. Recent remote-sensing of asteroids by Hayabusa2, OSIRIS-Rex, and Dawn spacecrafts as well as telescopic observations by AKARI infrared space telescope provided detailed IR reflectance spectra of asteroids [1–4]. These observations would allow us to constrain their paleo-aqueous environments.

This study aims to connect the observed IR spectra of asteroids to the original bulk compositions and T - P conditions of them or their parent bodies. We performed a series of chemical equilibrium calculations to obtain the mineral compositions. We computed the model IR reflectance spectra from the obtained mineral compositions. In this presentation, we compare the model results to the IR reflectance spectra of Ryugu, Bennu, Ceres, and the main-belt asteroids. We discuss their paleo-aqueous environments and the dynamic history of solar system.

Model: The chemical equilibrium calculations assumed the rocky bulk compositions of CV chondrites. We treated W/R as a parameter (0.2–10). We fixed the relative abundance of volatiles to water. Model 1 assumed a pure water and rock mixture. Models 2–4 assumed CO₂: 1, 3, and 10%, NH₃: 0.5%, and H₂S: 0.5% relative to water. The temperature T is a parameter and P equals the saturation vapor pressure of water. We used EQ3/6 computation software. In our model, pyrene represents organic phases, which would eventually form high-molecular-weight insoluble-organic-matter (IOM) typically found in meteorites.

The model IR reflectance spectra were calculated by adopting the radiative transfer theory for granular surfaces [5]. The refractive indices of endmembers were calculated from their reflectance spectra taken from RELAB database and [6, 7]. We computed single scattering albedo (SSA) of each endmember for an

assumed grain size (D), which is treated as a parameter. The reflectance of the mixture was calculated from the linear mixing of endmember SSAs. We employed the incident angle $i = 30^\circ$ and the emergence angle $e = 0^\circ$, respectively. We note that, though we carefully chose the endmember reflectance, the existing data sometimes contain the features caused by absorbed water on samples (e.g., at 1.4 μm and 1.9 μm in Figure 1).

Results: Model spectra show the dominance of OH-absorption at 2.7–2.9 μm due to abundant hydrous minerals (Figure 1). Addition of CO₂, NH₃, and H₂S leads to absorption at 3.1 μm and 3.4 and 4.0 μm , which are attributed to NH₄-saponite and carbonates, respectively (Figure 1a). As W/R decreases, carbonate absorption disappears and overall reflectance becomes lower because carbonates are converted into organics (CO₂-reduction) and magnetite dominates over organics eventually (Figure 1b). Decreasing W/R also causes the shift of OH-absorption to shorter wavelength because the dominant hydrous phases change from Fe-rich to Mg-rich. Ammonia-related absorption appears at limited W/R: W/R ~ 1 in Case 4 (Figure 1b) and W/R > 1 in Cases 2 and 3 (not shown), both at $T = 0^\circ\text{C}$. Raising T higher than 0°C also removes NH₄-absorption, whereas carbonate-absorption keeps existing (Figure 1c). Raising T also causes the shift of OH-absorption to longer wavelength as dominant hydrous phases change from Mg-serpentine to ferrosaponite and clinocllore for W/R ~ 1 (Figure 1c) or anhydrous minerals for W/R < 0.5 (not shown). Finally, increasing D darkens the overall reflectance (Figure 1d), as reported for natural samples [e.g., 8].

Discussion: Ryugu's IR reflectance spectra observed by The Near Infrared Spectrometer (NIRS3) onboard Hayabusa2 (1.8–3.2 μm) are very low (~ 0.02) and contain sharp absorption at 2.72 μm [1]. Our model assuming equilibrium chemistry excludes high T ($> 350^\circ\text{C}$) and high W/R (> 2) to reproduce the position by Mg-serpentine (Figures 1b and 1c). A large grain size ($D \sim 1\text{ mm}$) may be favored by the low reflectance (Figure 1d). The low T and large D may be consistent with the images taken by The Mobile Asteroid Surface Scout (MASCOT) lander, where inclusions are preserved and no fine-grained deposits are found [9].

Bennu's reflectance spectra observed by OSIRIS-REx Visible and InfraRed Spectrometer (OVIRS) showed the absorption near 2.7 μm [10]. Our model

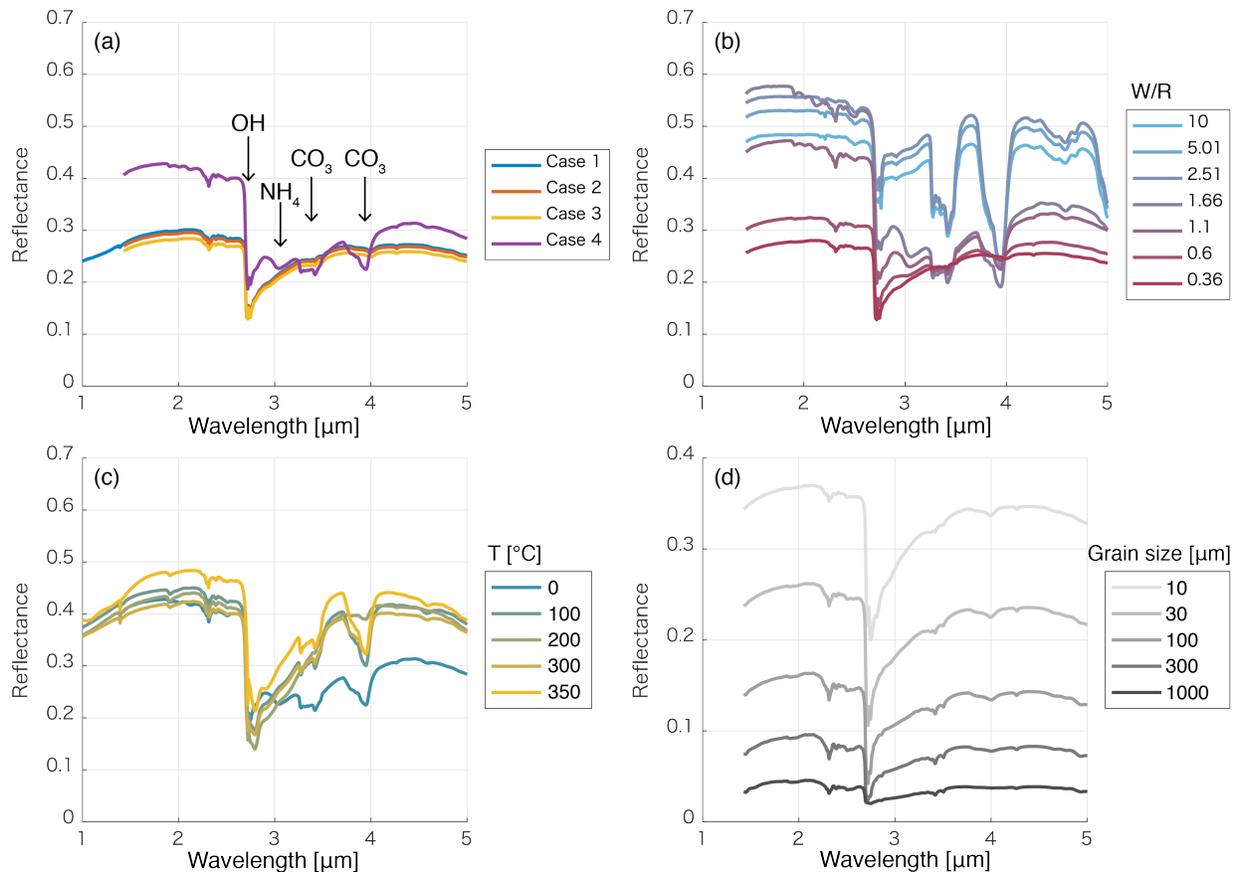


Figure 1. Model reflectance spectra. a: Comparison of Cases 1-4 ($T = 0\text{ }^{\circ}\text{C}$, $W/R = 1$, $D = 22.5\text{ }\mu\text{m}$). b: Dependence on W/R (Case 4, $T = 0\text{ }^{\circ}\text{C}$, $D = 22.5\text{ }\mu\text{m}$). c: Dependence on temperature (Case 4, $W/R = 1$, $D = 22.5\text{ }\mu\text{m}$). d: Dependence on grain size (Case 4, $T = 0\text{ }^{\circ}\text{C}$, $W/R = 0.2$).

again excludes high T ($> 350\text{ }^{\circ}\text{C}$) and high W/R (> 2) (Figures 1b and 1c).

For both Ryugu and Bennu, currently published data are insufficient to confirm the presence or absence of $3.1\text{ }\mu\text{m}$ absorption. If confirmed, it further constrains their parent bodies' conditions.

Ceres' reflectance spectra observed by Visible-Infrared Mapping Spectrometer (VIR) on the Dawn spacecraft showed absorptions at 2.7 , 3.1 , 3.4 , and $4.0\text{ }\mu\text{m}$, suggesting the presence of Mg-phyllosilicates, ammonia-bearing phases, and carbonates [3]. Our model constrains the condition to be $T \sim 0\text{ }^{\circ}\text{C}$ and $W/R \sim 1$ or higher (Figures 1b and 1c).

Finally, the IR reflectance spectra of the C-complex main-belt asteroids observed by AKARI show ~ 2.7 – $2.8\text{ }\mu\text{m}$, $3.1\text{ }\mu\text{m}$, and 3.4 and $4.0\text{ }\mu\text{m}$ absorptions, in order of detection frequency [4]. The origins of this trend would be the diversities of original compositions and of quenching temperature. Our model showed that, when the starting materials contain CO_2 , carbonate-absorption appears in a wide T range. Therefore, the presence or absence of 3.4 and $4.0\text{ }\mu\text{m}$

absorption is likely to be attributed to the variety of original compositions, for instance, due to the different formation locations in the protosolar nebula. In contrast, NH_4 -absorption appeared in limited conditions: $T \sim 0\text{ }^{\circ}\text{C}$ and $W/R \sim 1$ or higher. If the quenching temperature is the dominant factor, our model predicted that the $3.1\text{ }\mu\text{m}$ absorption is accompanied by OH-absorption at relatively short wavelength. On the other hand, if the original composition is the dominant factor, no such correlation would be observed. Future analysis of asteroids' spectra will distinguish the scenarios and unveil the formation and migration history of these bodies.

References: [1] Kitazato, K. et al. (2019) *Science*, 364, 272–275. [2] Hamilton, V. E. (2019) *Nature Astron.*, 3, 332–340. [3] De Sanctis, M. C. et al. (2015) *Nature*, 528, 241–244. [4] Usui, F. et al. (2018) *Publ. Astron. Soc. J.*, 71, 1–41. [5] Hapke, B. (2012) *Cambridge University Press*. [6] Ehlmann, B. L. et al. (2018) *Meteor. Planet. Sci.*, 53, 1884–1901. [7] Kaplan, H. H. et al. (2018) *GRL*, 45, 5274–5282. [8] Cloutis, E. A. et al. (2018) *Icarus*, 305, 203–224. [9] Jaumann, R. et al. (2019) *Science*, 365, 817–820.