Mid-infrared optical constants of clinopyroxene and orthoclase derived from oriented single-crystal reflectance spectra

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ABSTRACT

We have determined the mid-IR optical constants of one alkali feldspar and four pyroxene compositions in the range of 250–4000 cm⁻¹. Measured reflectance spectra of oriented single crystals were iteratively fit to modeled spectra derived from classical dispersion analysis. We present the real and imaginary indices of refraction (n and k) along with the oscillator parameters with which they were modeled. While materials of orthorhombic symmetry and higher are well covered by the current literature, optical constants have been derived for only a handful of geologically relevant monoclinic materials, including gypsum and orthoclase. Two input parameters that go into radiative transfer models, the scattering phase function and the single scattering albedo, are functions of a material’s optical constants. Pyroxene is a common rock-forming mineral group in terrestrial bodies as well as meteorites and is also detected in cosmic dust. Hence, having a set of pyroxene optical constants will provide additional details about the composition of Solar System bodies and circumstellar materials. We follow the method of Mayerhöfer et al. (2010), which is based on the Berreman 4 × 4 matrix formulation. This approach provides a consistent way to calculate the reflectance coefficients in low-symmetry cases. Additionally, while many models assume normal incidence to simplify the dispersion relations, this more general model applies to reflectance spectra collected at non-normal incidence.

Keywords: Spectroscopy, infrared measurements, planetary surfaces, mineralogy

INTRODUCTION

Pyroxenes are common rock-forming minerals in terrestrial planets and asteroids. They are also abundant in meteorites and interplanetary and cosmic dust particles. The pyroxene crystal structure allows for various cations to occupy its M1 and M2 sites, with ordering and preference between the two sites being controlled by temperature, pressure, and cooling rate. As a result, pyroxene composition is a good indicator of the thermal history of the source magma (Klima et al. 2008) and can be used to compare the evolution of different planetary bodies (Karner et al. 2006). Pyroxene is readily detected in the near-infrared (NIR) via two strong Fe²⁺ crystal field absorption bands near 1 and 2 μm whose positions and strengths are functions of composition. As the mid-IR (MIR, around 3–15 μm, although definitions vary) is sensitive to Si-O vibrational modes (Salisbury 1972), it can be used to provide additional details about composition as well as to estimate abundance relative to more felsic components (Ramsey and Christensen 1998).

The wavelength-dependent complex index of refraction (\( \tilde{n} = n + ik \)), where \( n \) and \( k \) are the optical constants, is an essential input into scattering models of planetary surfaces. Commonly used radiative transfer models of airless bodies include Lumme and Bowell (1981), Hapke (1993, 2012), Shkuratov et al. (1999), and Mishchenko et al. (1999). Hapke’s theory uses optical constants to calculate the single scattering albedo and the phase function. In Shkuratov’s model of lunar regolith scattering, the reflectance of the surface (\( A \)) depends on only four parameters \( A(n,k,S,q) \), where \( n \) and \( k \) are the optical constants, \( S \) is the scattering path-length, and \( q \) is the packing density (Shkuratov et al. 1999). Hence, accurate determination of optical constants for various minerals is necessary for using remote sensing data to make quantitative estimates of mineralogical composition. At MIR wavelengths, materials of orthorhombic symmetry and higher are well covered by the current literature; these include quartz, calcite, olivine, orthopyroxene, kaolinite, serpentine, palagonite, and iron oxides (Spitzer and Kleinman 1961; Wenrich and Christensen 1996; Lucy 1998; Lane 1999; Suto et al. 2002; Glotch et al. 2006; Sogawa et al. 2006; Dyar et al. 2009; Roush et al. 1991; Glotch and Rossman 2009).

Monoclinic and triclinic minerals have largely been ignored in optical constant research, although in some cases orientation-averaged effective optical constants have been calculated and presented (e.g., Roush et al. 1991; Glotch et al. 2007). This is due to the additional complexity of obtaining values for low-symmetry materials, despite the fact that these crystal systems contain important rock-forming mineral groups such as clinopyroxene and feldspar. In this work, we use dispersion analysis to calculate the optical constants of four distinct clinopyroxene compositions in the range of 250–4000 cm⁻¹, following the method of Mayerhöfer et al. (2010) and present a procedure that can be applied to derive the optical constants of monoclinic single crystals. We also calculate the optical constants of orthoclase and compare to the previously computed optical constants of Aronson (1986) as a test of our model.

BACKGROUND

The Moon

The Clementine mission provided a global lunar map of pyroxene abundance, broadly highlighting that it is a major component of the mare basalts and less prevalent in highlands. Modeled...