

IRON OPTICAL CONSTANTS AND REFLECTANCE SPECTROMETRY OF PLANETARY SURFACES.

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Introduction: Reflectance spectrometry is an important means for remotely obtaining information about the composition and physical state of planetary surfaces. Increased computing power and data storage capacity now permit sophisticated intimate mixture models based on radiative transfer physics [e.g., 1, 2, 3] to be applied to "spot" spectra and spectral imaging datasets having tens or hundreds of wavelength bands. Large numbers of model spectra can be computed and compared to the spectra of a remotely observed surface in order to determine the best-fit composition. In Hapke's formulation, the reflectance spectrum of a mixture is computed from single-scattering albedo spectra of the endmembers under consideration. Single-scattering albedo, w , is the probability that a photon incident on a regolith grain will be absorbed or scattered out of the beam, and is independent of illumination or viewing geometry. The single-scattering albedo in turn is a function of a grain's scattering behavior (e.g., degree of internal scattering) and absorption coefficient. The absorption coefficient is in turn governed by the material's complex index of refraction: $n_c = n + ik$ [4, 5], where n and k are called the optical constants, or real and imaginary parts of the index of refraction, and i is $\sqrt{-1}$. The optical constants are inherent properties of a material; variations along crystallographic axes in a particular mineral will be averaged when considering powdered samples or a regolith. The optical "constants" of a material do vary with frequency (wavelength), and one authority [6] has suggested that they instead be called "optical functions" to emphasize that they are a spectral quantity.

For transparent minerals and glasses, the optical constants can be calculated from reflectance spectra of powdered samples, as was done by [7] for olivine and pyroxene [see also 8].

Opaque metal can be present in planetary regoliths in two forms, "large" and nanophase. Coarse-grained metal (i.e., grains that are large compared to the wavelength of light) is found "native" in meteorites and lunar samples. Much smaller (nanometer to micrometer in size) metal blebs and coatings on and within regolith grains are produced in the process of space weathering, by reduction of ferrous iron in silicates and vapor deposition caused by solar wind sputtering and micro-meteorite bombardment [2, 9, 10]. The metal produced by space weathering is referred to as "nanophase iron"

(npFe⁰) or "submicroscopic metallic iron" (SMFe). Space weathering has strong effects on the optical properties of a regolith. Compared to the spectrum of a freshly powdered lunar rock, a mature lunar soil has a steeper ("redder") positive continuum slope, reduced overall reflectance, and greatly muted absorption bands [e.g., 11]. Hapke's [2] reflectance model includes a treatment of space weathering via the spectral effects of npFe⁰.

In order to model intimate mixtures containing opaque metal (in either or both of the coarse-grained or nanophase forms), the optical constants of the metal must be supplied. The optical constants of metals could be obtained from reflectance measurements, as for finding n and k of transparent minerals [7]. However, samples of terrestrial iron or iron meteorites may be altered by exposure to the moist terrestrial atmosphere [12], potentially producing coatings that could interfere with determination of the spectral properties of the unaltered metal. For this reason, some workers have elected to use values for n and k of iron from the applied physics and materials science literature. For example, [2, 13, 14, 15] used the iron optical constant values of [16], and a group at the University of Hawaii [17, 18, 19] has recently been using those of [20].

In addition to [16] and [20], optical constants of iron have been reported or compiled by [21, 22, 23]. The data are plotted in Figure 1. There are a number of shortcomings associated with use of these published values for planetary reflectance modeling, including wavelength range, spectral resolution, and consistency. For example, [16] gave values between 0.1 and 1.93 μm , heavily weighted toward the ultraviolet (UV), with only 15 of 49 data points longwards of 0.50 μm . [21] provided data at 20 wavelengths between 0.67 and 5.0 μm . [23] presented the data of [21] between 1.0 and 5.0, the [24] data in the vacuum ultraviolet (40 wavelengths 0.10 - 0.25 μm), and no values between 0.25 and 1.0 μm . [20] reported n and k at just 10 wavelengths between 0.12 and 5.0 μm , 7 of which are at <0.6 μm . [22] made measurements of n and k at a single wavelength (0.63 μm) and found values that are considerably higher than those of other workers. The often-used [16] data differs substantially from that of [20]. As Fig. 1 illustrates, there is no single dataset that covers the entire wavelength range of interest to plane-

tary reflectance spectroscopy (UV to mid-IR) with high spectral resolution over the entire range.

New Measurements: We have initiated a program to make new measurements of the optical constants of high-purity iron films. We employ modern variable-angle spectroscopic ellipsometers at the National Institute of Standards and Technology's Semiconductor Electronics Division. Ellipsometry involves measurement of the change in polarization of light reflected from the surface of a sample. A collimated beam of monochromatic linearly polarized light is directed at a sample, and the polarization state of the elliptically polarized reflected light is analyzed. Because the technique depends only on measurement of the ratios of two values (incident and reflected *s*- and *p*-polarization intensities), it is highly accurate and reproducible even at low light levels and is not susceptible to variations in lamp intensity or the "purge" (exact pressure of the inert gas used to fill the sample chamber during measurement). These ratios are related to the optical properties of the ambient-sample interface through the electromagnetic theory of reflection. The parameters of interest are determined by solving the inverse problem. In spectroscopic ellipsometry (SE), these measurements are made at a range of wavelengths.

Ellipsometry measures a relative change in polarization as light reflects from or transmits through a material structure. The measured response depends on the optical properties and thickness of individual materials. Thus, ellipsometry is primarily used to determine optical constants of a simple substrate as well as film thicknesses and optical constants of individual layers within a stack of multiple layers. However, it is also applied to characterize composition, crystallinity, roughness, doping concentration, relative film or bulk material density, and other material properties associated with a change in optical response.

Since SE is sensitive to monolayers on the sample surface, especially in the spectral range of strong absorptions, our approach to obtain a bulk-like optical function of the metal is to minimize the surface effects (e.g., roughness, native oxides) and optimize the vacuum deposition of our metal films samples. Furthermore, other physical and chemical characterization tools will be used to evaluate structural and chemical properties and correlate them with the measured optical functions and the deposition conditions. The objective is eventually to obtain a set of optical functions that best represent the bulk values of the metal.

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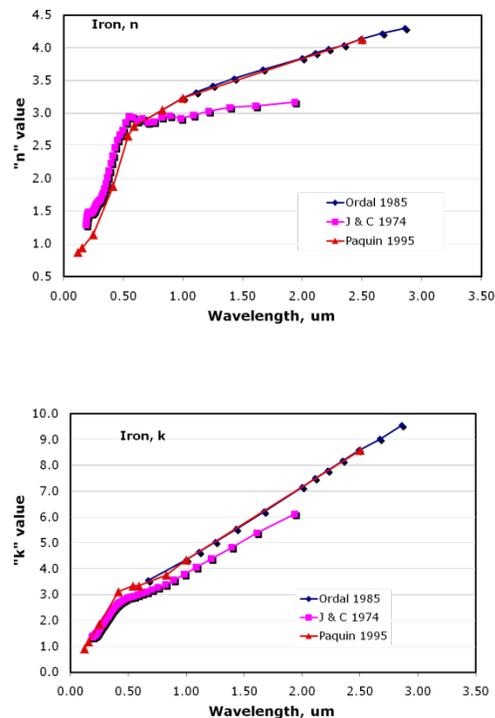


Figure 1. Optical constants of iron. Three examples from the literature are shown. [22] reported $n = 3.48$ and $k = 3.42$ at $0.633 \mu\text{m}$.