RELATIONSHIPS BETWEEN THE OPTICAL CONSTANTS AND SPECTROSCOPIC FEATURES OF PARTICULATE QUARTZ. IMPLICATIONS FOR REMOTE SENSING OF PLANETARY SURFACES;

Gabriele E. Arnold, Janice L. Bishop, Karin Junghans and Ulrich Schade; DLR, Institute for Planetary Exploration, Planetary Physics Section, Rudower Chaussee 5, 12489 Berlin, Germany.

Infrared reflectance spectra of particulate mineral samples depend on particle size and porosity. Analysis of remotely sensed infrared spectroscopic data requires the study of particle size effects on the spectral properties. Therefore, reflectance spectra of quartz size separates and the optical constants n and k have been measured. The relationships between spectral features, the optical constants and the Mie single scattering efficiencies are discussed. Variation of spectral features as a function of the particle size in relation to the optical constants allows us to identify at least 4 different cases of scattering and absorption behavior: (1) n=1, k is small, (2) k is large, n undergoes rapid change in the range of anomalous dispersion, (3) n < 1, k is low and (4) k is low and n >1.

Introduction. Many terrestrial planetary surfaces are covered with fine-grained particles below 50 µm (regolith). The effects of particle size on the reflectance spectra of terrestrial minerals have been discussed by Hunt and Vincent (1), Conel (2) Aronson and Emslie (3) and Salisbury et al. (4). Recently Moersch and Christensen(5) compared scattering models with reflectance spectra of quartz size separates and grouped spectral features on the basis of optical constants from Spitzer and Kleinman (6). We measured reflectance spectra for several particle size fractions of well-characterized quartz and classified the spectral features according to the the behavior of the optical constants measured using spectroscopic ellipsometry. Particle size effects are discussed in relation to the Mie efficiency factors, calculated from the optical constants.

Method. The reflectance spectra were performed using a Bruker IFS 88 Fourier transform spectrometer equipped with a Harrick reflectance attachment (7,8). The optical constants are determined by photometric ellipsometry of solid material and pressed pellets of fine-grained powder. This method allows us to obtain the refractive index for both ordinary and extraordinary directions from polarized reflectance measurements at multiple angles of incidence (9). Using a phase retarder we can measure the ellipsometric angles, which describe the amplitude relation and the difference of ordinary and extraordinary phases, respectively. The pellets were pressed in a hydraulic press with a pressure of 1 kbar on a 13-mm die.

Results and discussion. Reflectance spectra of quartz particle size separates are shown in Fig. 1 in the range between 7.0 and 12.5 µm. The corresponding reflectance and emittance spectra of these samples are shown from 4 to 18 µm in (8). Fig. 2 demonstrates the optical constants of a solid quartz sample and a pressed pellet of fine-grained material. The pressed material is a binary system of quartz and air, resulting in values of n

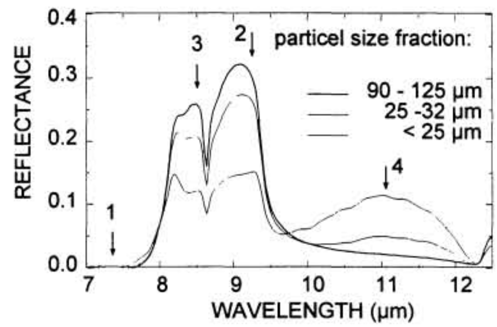

Fig. 1: Reflectance spectra of quartz particle size fraction

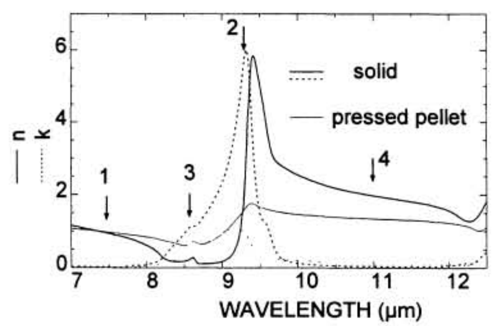

Fig. 2: Optical constants N = n + *i* k for solid quartz and pressed quartz pellets

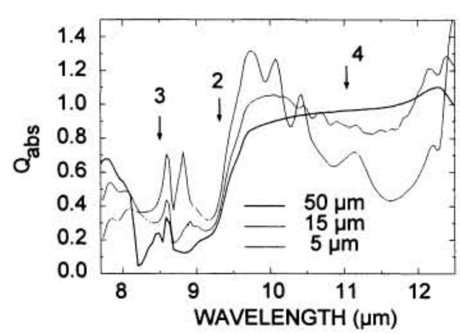

Fig. 3: Mie absorption efficiency factor for three particle radii

OPTICAL CONSTANTS AND SPECTROSCOPIC FEATURES; Arnold G. E. et al.

and k that do not reach the magnitudes of n and k for the quartz bulk material. Fig. 3 shows the Mie absorption efficiency factors for 3 corresponding particle radii calculated with the n and k values of the solid quartz. When comparing R, n, k and Q_{abs}, the several patterns of scattering and absorption behavior are observed as a function of particle size at different wavelengths.

Case 1: When n = 1 and k is low minimal scattering and absorption occur. The material is highly transparent here, resulting in minimum reflectance. The reflectance does not depend on the particle size of the sample when k = 0. This takes place at the short wavelength flank of the absorption bands, the strongest of which is called the Christiansen feature (at 1350 cm^{-1} for quartz (4)).

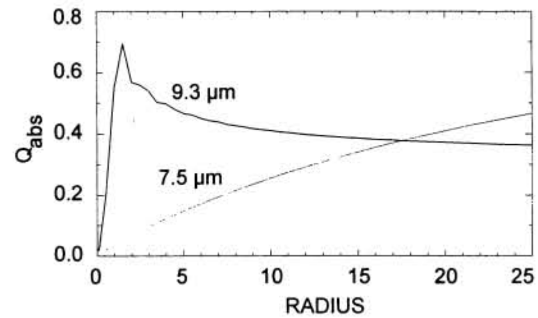

Fig. 4: Mie Absoption efficiency factor as a function of the particle radius

Cases 2 and 3: Where n and k undergo rapid change, the fundamental vibration band appears. For quartz this is a doublet near 1200 and 1100 cm^{-1}. The long wavelength peak of this band is observed at high k values (between maximum k and n values, *case 2*). For n < 1 and k still low (*case 3*) attenuated total reflection (ATR) relative to air takes place. This results in a reflectance peak at about 8 μm on the short wavelength flank of maximum k. Here the reflectance decreases with decreasing particle size, similar to the behavior discussed in case 2.

Case 4: When k is low and n > 1, the scattering efficiency of single particles increases with decreasing particle size, resulting in increased reflectance. This is observed for quartz near 11 μm and called the transparency feature (4). The absorption efficiency factor shows a local minimum at 11-11.5 μm for 30-μm-size spheres and at 11.5 μm for 10-μm-size spheres. This effect is especially notable for particle sizes < 25 μm (10). Fig. 4 shows the absorption efficency factors as functions of particle size for 7.5 μm and 9.3 μm. For large k the absorption efficiency increases with decreasing particle size (down to < 2 μm), resulting in a lower reflectance (Fig. 4, 9.3 μm). In contrast, in the case of small k values, Q_{abs} decreases with decreasing particle size for all grain sizes (Fig. 4, 7.5 μm). Therefore, the reflectance increases here.

Conclusion. These experiments show that the variation of spectral reflectance features with particle size can be classified in relation to the optical constants and single scattering characteristics of the material. In the case of large k (near 9.3 μm for quartz) the absorption efficiency increases with decreasing particle size (down to < 2 μm). At about 8 μm, where n < 1 and k is small, ATR results at the short wavelength peak of the doublet quartz fundamental. The reflectance decreases here if particle size is reduced. For low k values, Q_{abs} decreases and reflectance increases with decreasing particle size. Where n > 1 and k is small the material becomes more transparent (at 11 μm for quartz). The material neither scatters nor absorbs if n = 1 and k is nearly 0 (Christiansen frequency, about 7.4 μm for quartz). Radiative transfer models are being performed in order to analyze the shift of spectral bands and other spectral variation in more detail.

Acknowledgments: We would like to thank A. Roeseler for assistance with the ellipsometry measurements.

References.(1) Vincent R.K. and Hunt G. (1968) *Appl. Optic 7*, 53. (2) Conel J. E. (1969) *J. Geophys. Res. 74,* 1614. (3) Aronson J.R. and Emslie A.G. (1973) *Appl. Optics 12,* 2573. (4) Salisbury J.W. (1993) in *Remote Geochemical Analysis,* Eds. Pieters and Engert, Cambridge Univ., 79. (5) Moersch J.E. and Christensen P.R. (1995) *J. Geophys. Res. 100,* 7465. (6) Spitzer W.G. and Kleinman D.A. (1961) *Phys. Rev. 121,* 1324. (7) Arnold G.E. *et al.* (1995) *LPSC, LPSXXVI,* 53. (8) Arnold G.E. *et al.* (1996) *LPSC XXVII*, submitted. (9) Röseler A., (1990), *Infrared Spectroscopic Ellipsometry,* Akademie Verlag, Berlin. (10) Mustard J. *et al.* (1996) submitted to Icarus.