TEMPERATURE DEPENDENCIES OF CRYSTAL FIELD TRANSITION ENERGIES AND THEIR EFFECT ON THE MINERALOGICAL MAPPING OF THE LUNAR SURFACE.


Crystal field electronic transitions in the visible and near infrared regions form the basis of remote-sensing for mapping the mineralogy of the moon's surface [1]. Based on calibrations of band maxima for terrestrial minerals, the mineralogy in specific regions of the lunar surface has been deduced from reflectance spectra measured through earth-based telescopes [2,3]. Among the minerals used for mapping the lunar surface, pyroxenes and olivine are two of the most important because of their high abundance. Pyroxenes and olivine give characteristic crystal field bands centered near 1 micron due to six-coordinated Fe$^{2+}$ [4]. In addition to the 1 micron band, pyroxenes also give rise to another characteristic crystal field band located near 2 microns. The positions of the 1 micron bands for different compositions have been used to interpret the measured reflectance spectra of the lunar surface [5,6]. Previous interpretations are based on calibrations of crystal field bands at room temperature. However, the remote-sensing measurements are made on heated surfaces of the moon, which may attain temperatures of up to 130°C when irradiated by sunlight. There may be discrepancies in these mineralogical analyses because of the possible shift of crystal field bands with temperature. Thus, in this abstract we report some preliminary data on temperature dependencies of the crystal field bands for orthopyroxene and olivine, and assess their effect on the mineralogical mapping of the lunar surface.

We have designed sample holders which have allowed us to measure both transmitted absorption spectra and diffuse reflectance spectra of enstatite and forsterite at temperatures up to 400°C. The transmitted spectra were polarized and measured on oriented single crystals. The reflectance spectra were measured on powdered samples of approximately 100μm grain size. Negligible sample degradation was observed below 400°C. Although the crystal field bands broaden with heating, their intensities do not change significantly in this temperature range. The peak position of crystal field bands in the near infrared region as a function of temperature is shown in Figure 1. It is noted that the major 1 micron crystal field bands for enstatite and forsterite (γ-polarization) do not shift significantly with temperature. The two crystal field bands in the β-polarization of forsterite do shift rapidly towards lower energy with increasing temperature due to increasing distortion in the M1 site [7]. However, these two bands have smaller intensities and may be obscured by the stronger center peak at 1 micron (γ-polarization) in the unpolarized reflectance spectra from the lunar surface. The 2 micron band of enstatite also seems to show large temperature dependence. It may shift slightly toward lower energy at a temperature between 100 to 200°C and then move rapidly toward higher energy with further temperature increase. Because of the absorption by water vapor in the earth's atmosphere, the 2 micron band of pyroxenes is difficult to obtain through earth-based telescopes and thus has not yet been used for mapping the mineralogy of the lunar surface. However, the 2 micron band plays a prominent role in calibrations of pyroxene structure types and compositions obtained from reflectance spectra of returned lunar

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samples [5,6]. The shift of the 2 micron band with temperature may cause a large uncertainty in determining the pyroxene composition. For example, if our measurements are correct, the red shift of the 2 micron band in orthopyroxene at 200°C may be equivalent to an increase of FeSiO₃ content of ten mole percent or more. Thus, the temperature dependence of the 2 micron band must be documented for future spacecraft-based remote sensing measurements of the surfaces of the moon, Mercury, Mars, and the asteroids.

The mapping of pyroxenes and olivine on the lunar surface is mainly based on the major 1 micron bands which have been shown to be nearly independent of temperature below 400°C. This fortuitous result is consistent with the observation that compositions of pyroxenes predicted by remote-sensing agree with analyzed compositions of returned lunar samples [5,6]. The temperature dependence of crystal field bands and their effect on the mineralogical mapping of the lunar surface for glass, plagioclase, and ilmenite is yet to be determined and work is in progress in this direction.

References

Figure Caption
Figure 1. Band maximum as a function of temperature for enstatite (circles) and forsterite (triangles). Open and solid symbols are for transmitted absorption spectra and diffuse reflectance spectra, respectively. The compositions of enstatite are different in these two measurements. The direction of polarization for transmitted absorption spectra is indicated.