EFFECTS OF COMPOSITIONAL VARIATION ON ABSORPTION SPECTRA OF LUNAR PYROXENES. R. M. Hazen, P. M. Bell, and H. K. Mao, Carnegie Institution of Washington, Geophysical Laboratory, 2801 Upton St., NW, Washington, DC 20008.

Absorption bands of pyroxenes dominate visible and near-infrared reflectance spectra of lunar materials (1). Positions and intensities of pyroxene absorption features are sensitive to composition, and observed reflectance spectra, therefore, may be related to average pyroxene composition. Interpretation of diffuse reflectance spectra must be based, in part, on correlations between composition and absorption spectra of minerals. Features of single-crystal polarized absorption spectra of pyroxenes have been reported by many investigators (2). Variations have been noted among spectra from pyroxenes of different compositions, but the quantitative nature of these variations has not been completely documented. Controversy exists over the origin of several absorption features, and little attention has been devoted to the effects of zoning, exsolution, or cation ordering on the spectra of pyroxenes. In this study we report quantitative variations of pyroxene absorption spectra with composition, zoning and exsolution.

Polarized absorption spectra of fifteen lunar pyroxenes and synthetic orthoferrisilite, FeSiO$_3$, were measured on polished, oriented single crystals using techniques of Mao and Bell (3). Compositions of these specimens and eighteen previously described pyroxenes are distributed over much of the pyroxene quadrilateral, and have significant chromium (0.0 to 1.5% Cr$_2$O$_3$) and titanium (0.0 to 5.3% TiO$_2$) variations as well.

Major features in all lunar pyroxene spectra are intense absorption bands at 1 µm and 2 µm, a sharp peak or doublet at 505 nm, and an intense absorption edge below 700 nm. Additional weaker peaks in the visible region of many pyroxene spectra are peaks at 425 and 550 nm, and broad absorption maxima at 460-480 and 630-660 nm. The absorption spectrum of FeSiO$_3$ provides unambiguous assignment of features due to Fe$^{2+}$ in octahedral coordination. Maxima at 1 and 2 µm, and 430, 460-480, 505, and 550 µm are observed in the ferrosilite spectrum and are, therefore, assigned to Fe$^{2+}$ crystal field effects (4).

Systematic variations in the positions of the 1 and 2 µm bands with composition, as projected onto the pyroxene quadrilateral, are illustrated in Fig. 1, which agrees with previous semi-quantitative plots (5,6). The energy of these bands decreases with increasing Fe and Ca; addition of calcium and iron to enstatite increases the size, and alters the distortion, of octahedral sites, thus lowering the transition energy.

The broad band at 640 nm has been assigned variously to Fe$^{3+}$ (7), titanium (2), and Cr$^{3+}$ (8). The intensity of this band correlates well with Cr$^{3+}$ (Fig. 2), but not with iron or titanium.

The sharp peak at 505 nm is a doublet in most low-calcium pyroxenes, but a singlet in augites. This difference is ascribed to the lower symmetry of the M1 site in pigeonites and orthopyroxenes, compared to augites. The position of the 505 nm peak varies from 504 nm near enstatite to 511 nm near hedenbergite, in a manner similar to that illustrated in Fig. 1.

Intensity of the broad maximum at 460-480 nm correlates with titanium (2) but the peak is also observed in pure FeSiO$_3$. This feature is, therefore, attributed to a superposition of iron and titanium absorption effects. The slope of the absorption edge below 700 nm also correlates well with titanium variation.
ABSORPTION SPECTRA OF LUNAR PYROXENES

Hazen, R. M. et al.

Figure 1. Positions of the 1 and 2 μm absorption maxima vs. composition, projected onto the pyroxene quadrilateral. Solid lines = 1, dashed = 2 μm.

(calculated as TiO₂), illustrated in Fig. 3. This supports calculations which ascribe the absorption edge to complex charge transfer effects, primarily from Ti⁴⁺-Fe²⁺ (9).

Pyroxene absorption features in diffuse reflectance spectra, including the 1 and 2 μm bands and the absorption edge, are dependent on variation of Fe, Ca and Ti. Information on pyroxenes, combined with systematic studies of other extraterrestrial materials, should provide a more quantitative basis for interpreting reflectance spectra of remote objects.