Complex Quartz/Kaolinite Scattering in the TIR

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This note deals with the interpretation of complex spectra that can occur with mixtures of quartz and kaolinite. I suggest that these spectra arise when kaolinite and/or quartz exists as optically thin material on optically thick quartz and develop a non-linear model that explains the effects that are seen.

Introduction

Figure 1 shows five examples of such spectra with varying amounts of anomalous behaviour. The top spectrum shows a relatively normal quartz spectrum with an anomalous sharp nick ~9 μm due to kaolinite. This spectrum is seen in many quartz-rich rocks with very small amounts of kaolinite. (Sometimes the kaolinite may not even be detected in the SWIR). More severe distortions, like those below, are less common and are usually associated with badly weathered or heavily altered samples

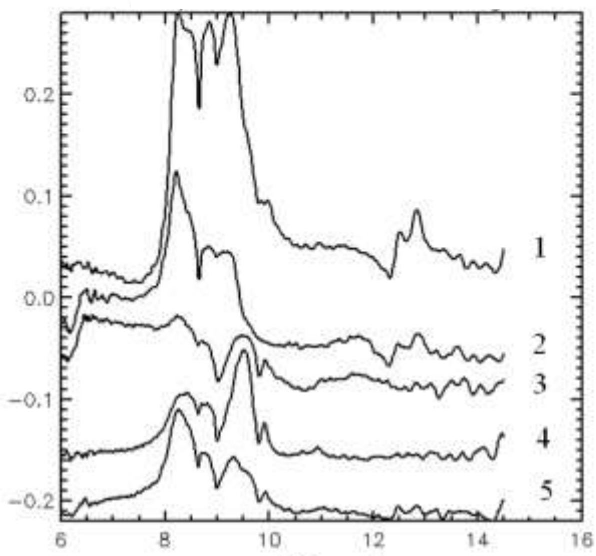

Figure 1

Salisbury et. al.[1] also found this spectrum in studies of soil samples. Figure 2 is reproduced from their paper. In each figure the dotted curve was obtained when thin coatings were placed on pure quartz (the full curve).

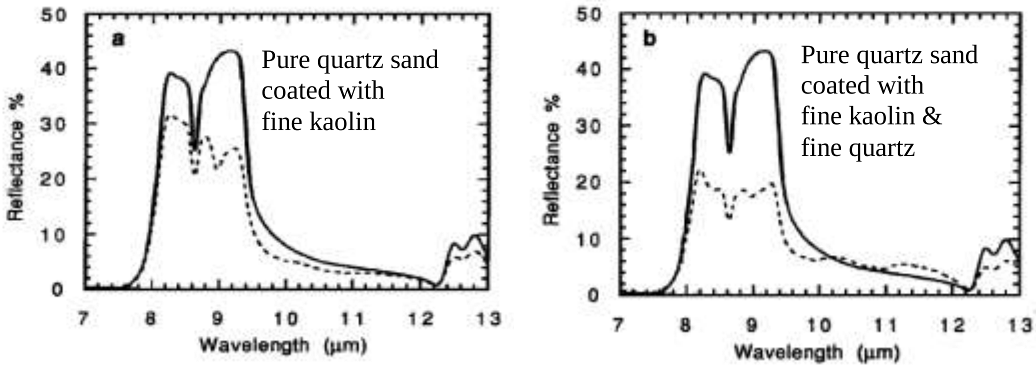

Figure 2

They conclude …

> "From these reflectance measurements, we believe that we have demonstrated that the spectral behaviour of our soil samples … can be explained in essence by reflectance from an optically thick quartz substrate combined with transmission through very fine grained, optically thin, particulate coatings of kaolinite mixed with varying amounts of similarly fine quartz."

In Figure 2a you can see that, in addition to lowering the overall quartz reflectance pattern, the major effect of kaolinite is to create the feature at ~9 μm. When both fine quartz and kaolinite are present

[1] Thermal-infrared remote sensing and Kirchhoff's law 1. Laboratory measurements Salisbury et al, JGR 99, No. B6, p 11,897-11,911.

(Figure 2b) there is an additional change to the shape of the short wavelength quartz feature around 8.4 μm. This effect, on its own, is also common in HyLogger data.

Our standard linear methods do not model these spectra adequately. Figure 3 shows the result of modelling spectrum 5 from Figure 1 as a linear combination of quartz and kaolinite ($0.94\rho_q + 0.06\rho_k$). It does not explain the data because a more complex, non-linear model is required to explain the process proposed by Salisbury et. al.

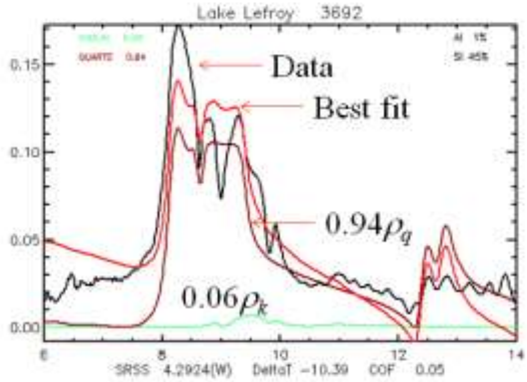

Figure 3

A Non-linear Model

Once we consider the possibility that there may be optically-thin surface layers of quartz and/or kaolinite on optically thick quartz we need to consider the transmission spectra of these materials as well as their reflectance. In the following I will model the surface being measured as made from three components.

1. Optically-thick kaolinite that reflects in the normal way. (shown in mauve in figure 4).
2. Optically-thin quartz on optically thick quartz which results in the transmission spectrum of quartz superimposed on the reflectance spectrum of quartz. (shown in orange)
3. Optically-thin kaolinite on optically thick quartz which results in the transmission spectrum of kaolinite superimposed on the reflectance spectrum of quartz. (in green)

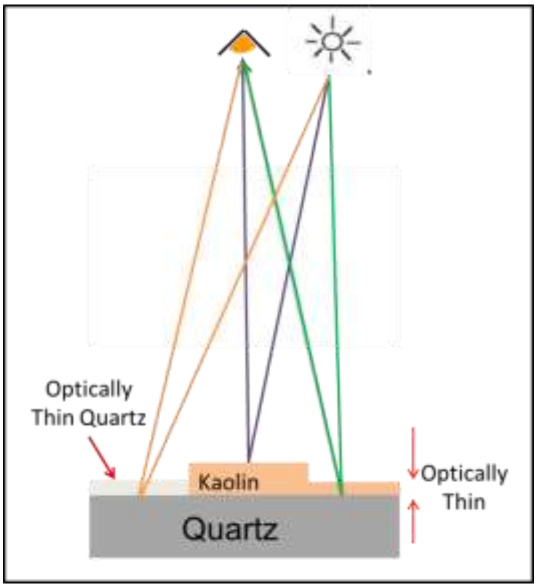

Figure 4

If ρ_k and t_k are the reflectance and transmittance spectra of kaolinite and ρ_q and t_q are the reflectance and transmittance spectra of quartz. Then we can write the reflectance of the sample as

$$\rho = B + w_k \rho_k + w_{qq}\rho_q t_q + w_{kq} \rho_q t_k \quad (1)$$

Here w_k , w_{qk} , and w_{qq} are weights related to the amount of each of the three components described above and B is a (hopefully smooth) background spectrum to model slowly varying reflectance changes with wavelength. Of course the transmission terms t_k and t_q will depend on the thickness of the optically thin components will change from sample to sample. To cope with this we need to define them in terms of reference transmission spectra τ_k and τ_q for kaolinite and quartz, so that:

$$t_q = \tau_q^{d_q} \text{ and } t_k = \tau_k^{d_k}$$

where d_q and d_k allow us to parameterize the thickness of the optically thin components. For example, if $d_q = 2$ this implies that the actual sample has twice the optical thickness of quartz relative to the reference transmission measurement.

Substituting into (1) gives:

$$\rho = \underbrace{B}_{\text{Background term}} + \underbrace{w_k\rho_k}_{\text{Standard kaolinite reflectance}} + \underbrace{w_{qq}\,\rho_q\tau_q^{d_q}}_{\text{Quartz seen through optically thin quartz}} + \underbrace{w_{kq}\,\rho_q\tau_k^{d_k}}_{\text{Quartz seen through optically thin kaolinite}}$$

In this work the background spectrum B is modelled in terms of Chebychev Polynomials[2] T_i for $i = 1, 2, ..n$ which form an orthogonal basis set of smooth functions over the wavelength interval. Thus

$$B = \sum_{i=1}^{n} b_i T_i$$

In general $3 \le n \le 7$.

We now have a non-linear model for the reflectance of the sample in terms of two reference reflectance spectra (ρ_k and ρ_q), two reference transmission spectra (τ_k and τ_q), five unknown parameters (w_k , w_{qq} , w_{kq}, d_q and d_k) and n background coefficients which will change from sample to sample.

Using the Model

The four reference spectra used here are shown in figure 5. Note the transmission minimum at 9.0 μm in the kaolinite transmission (red) that causes the nick seen in spectrum1 and in the Salisbury data.

Note also how the main kaolinite transmission minimum is displaced from the 9 μm quartz feature so that its effect is not very noticeable in comparison with the weaker kaolinite feature at shorter wavelength.

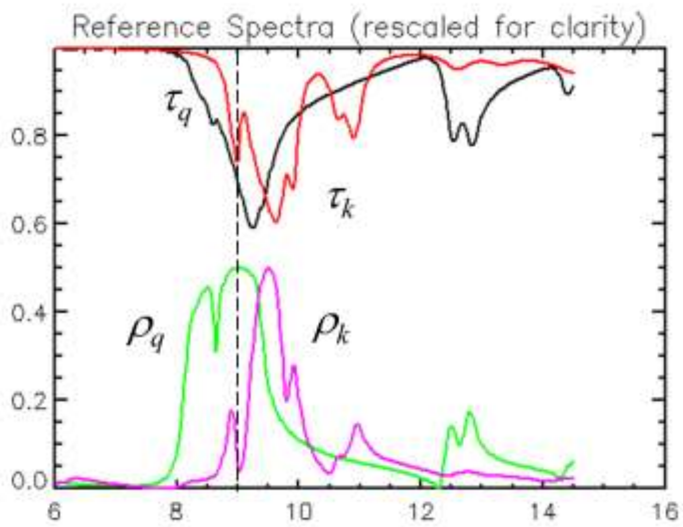

Figure 5

[2] https://en.wikipedia.org/wiki/Chebyshev_polynomials

When this this model is fitted to Spectrum 1 using an iterative non-linear solver[3] implemented in IDL, we get the results shown in figure 6.

In the top panel

- The data is plotted in black and
- The fit to the model in red.
- The mauve is the component of the fit that has undergone standard reflectance from optically thick kaolinite. ($w_k \rho_k$)
- The orange shows the component that has been transmitted twice through the optically thin quartz ($w_{qq} \rho_q t_q$)
- The green the component that has been transmitted twice through the optically thin kaolinite. ($w_{kq} \rho_q t_k$)

In the lower panel

- The data is again plotted in back,
- The kaolin transmittance t_k in green
- The quartz transmittance t_q in orange.
- The background B is plotted in red.

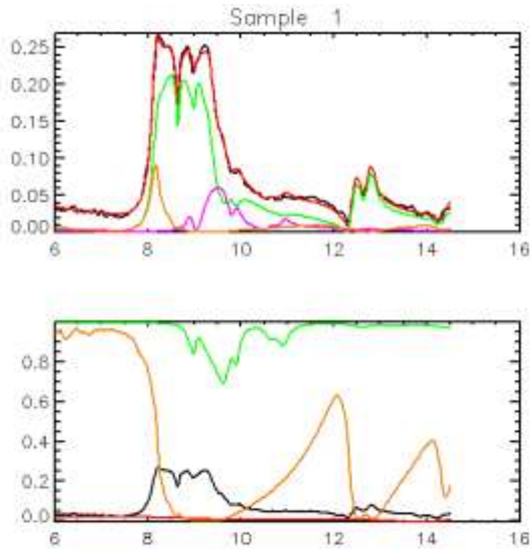

Figure 6

The optically thin kaolinite (upper green) is the major component in this model. Its spectrum is basically that of quartz where the effect of the kaolinite is to introduce the nick at 9 μm and to “shave-off” some to the long-wavelength side of the 9μm quartz feature.

The optically thin quartz component (upper orange) shows the effect of very strong absorption by the optically thin quartz (see quartz transmission: lower orange). It is so strong that only the short wavelength side of the 8 mm quartz feature remains. This feature is common in much HyLogger data and can cause a pronounced sharp spike at this wavelength.

The effect of the standard kaolinite (upper mauve) reflectance is to “replace” some of the reflectance that has been “shaved-off” the quartz spectrum in the optically thin kaolinite component.

The background spectrum (lower red) is quite smooth and low amplitude.

[3] Lasdon, L.S. and Waren, A.D., "Generalized Reduced Gradient Software for Linearly and Nonlinearly Constrained Problems", in "Design and Implementation of Optimization Software", H. Greenberg, ed., Sijthoff and Noordhoff, pubs, 1979.

The results for Sample 2 are shown in figure 7. They are presented in the same format as figure 5. Even though there is a slight nick in the data at 9 µm the the model has missed this and has not incorporated any kaolinite at all. Thus there are only two components. The first is an unmodified quartz spectrum (green) because the the model has chosen the optically thin kaolinite to be so thin it is non-existant. The second is an optically thin quartz response (orange). The background (red) is rather less smooth than for sample 1 to accommodate the absorption feature at ~6.1 µm which is probably caused by water in the sample.

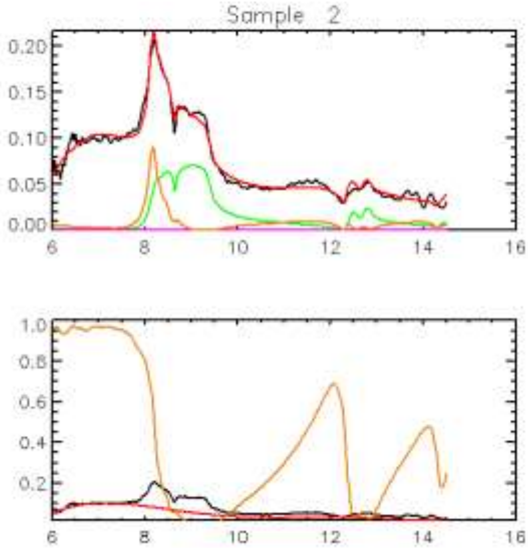

Figure 7

The results for Sample 3 are shown in figure 8. This sample is dominated by standard kaolinate reflectance and optically thin quartz. Except at short wavelength all the quartz restrahlen signature is hidden by strong quartz and kaolinite absorption. Again, the background it accomodating a strong water feature at 6.1 µm.

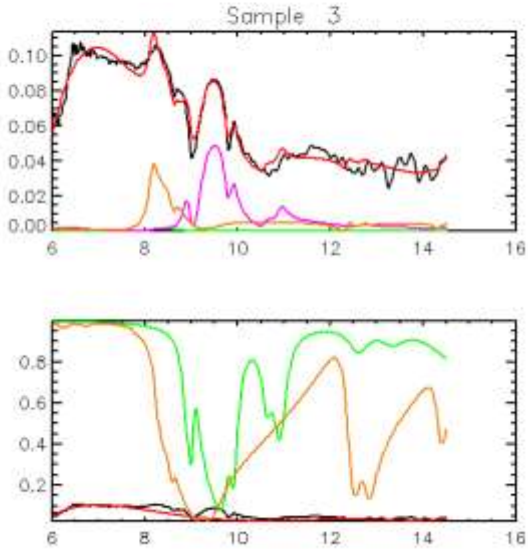

Figure 8

The results for Samples 4 and 5 are shown in figure 9. Sample 4 is also dominated by standard kaolinite reflectance but there are roughly equal contributions from the three effects in sample 5

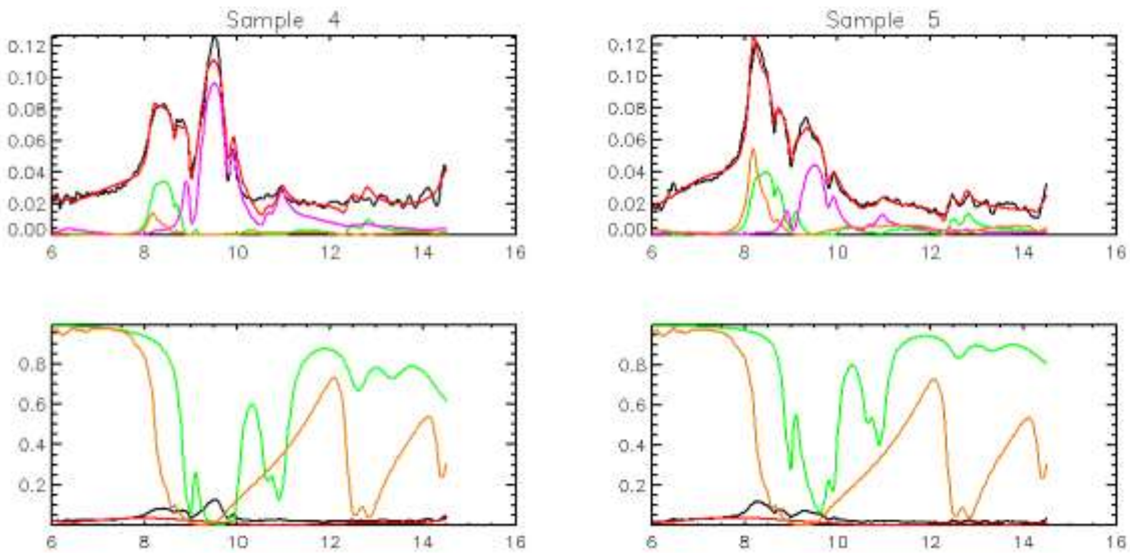

Figure 9

Conclusions

In spite of its simplistic form, this model explains these difficult spectra quite well. However, just because it provides a reasonable explanation of some very difficult spectra, it cannot be assumed that it is complete or even correct. No one who has seen an electron micrograph of the broken surface of a typical rock could believe that the simplistic geometry of figure 4 in any way represents reality. It is possible that some other combination of the properties of quartz and kaolinite will model the data equally well. More modelling should be done using conventional volume scattering theory to see if it can reproduce the same spectral features.

The non-linearity of the model means it probably is computationally too slow to incorporate into linear algorithms such a TSA or jCLST but there may be suitable ways of linearizing the problem to be compatible with these algorithms.

We also need to think about how other optically-thin coatings of minerals will respond with quartz.

Much more needs to be done on this issue.