Caractérisation des sols par l’analyse d’images hyperspectrales en télédétection

A Study on Hyperspectral Remote Sensing Data Processing and Analysis applied to 3D Mineral Mapping

Jinnian Wang

Thèse de Doctorat en Informatique

Directeur de thèse : Dr. Jean Sequeira

Aix-Marseille Université

Ecole Doctorale Mathématique et Informatique (ED 184)

Laboratoire LSIS (UMR CNRS 7296)

Jury :

M. Gilles Gesquière – Professeur, Université Lumière Lyon II
M. Franck Marzani – Professeur, Université de Bourgogne – Rapporteure
M. Sébastien Mavromatis – Maitre de Conférence, Aix-Marseille Université
M. William Puech – Professeur, Université de Montpellier II – Rapporteur
M. Jean Sequeira – Professeur, Aix-Marseille Université (Directeur de thèse)
Mme Sophie Viseur – Ingénieur de Recherche, Cerege, Aix-Marseille Université

Soutenance, le 31 Octobre 2014
ABSTRACT

A Study on Hyperspectral Remote Sensing Data Processing and Analysis applied to 3D Mineral Mapping

Hyperspectral remote sensing has been used successfully to identify and map abundances and compositional difference of mineral groups and single mineral phases. This research will toward developing a 3D mineral mapping system that integrate surface (airborne and satellite) and subsurface (drill core) hyperspectral remote sensing data and carries it into quantitative mineral systems analysis. The main content and result is introduced as follows:

• For Surface mineralogy mapping, we have developed and optimized the processing methods for accurate, seamless mineral measurements using Airborne and Satellite hyperspectral image. This requires solutions for unmixing background effects from target minerals to leave residual scaled mineral abundances equivalent to vegetation-free pixels. Another science challenge is to improve the atmospheric correction. Also Hapke BRDF model is used on the study in the linear and nonlinear mineral spectral mixing models, and developing unmixing algorithms based on spectral libraries, the position, depth and shape of selected absorption features in the visible-near (VNIR), shortwave (SWIR) and thermal infrared (TIR) for mineral mapping.

• For the subsurface mineralogy mapping, we have developed Field Imaging Spectrometer System (FISS) and Drill Core Logging for the subsurface mineralogy mapping, the Key science challenges will be establishing the accuracy of derived mineral products through associated laboratory analysis, including investigations from SWIR into the thermal infrared for measuring minerals.

• The 3D mineral maps derived from hyperspectral methods can distinctly improve our understanding of mineral system. We use GIS system integrating surface and subsurface mineralogy mapping, with 3D mineral models for demonstration exploitation of economic mineral deposits in test site.
My Publications Related to This Thesis


Jinnian Wang, Lifu Zhang, Jun Yan and Qingxi Tong (2011) “A new ground-based hyperspectral sensor system, A novel field imaging spectrometer improves the efficiency of field measurements while obtaining fine spatial and spectral information”, SPIE Newsroom. 20 September 2011 DOI: 10.1117/2.1201108.003774


Some of my previous academic activities in this field

My research focus on hyperspectral remote sensing technology and applications since I had worked in Chinese Academy of Science (CAS) in 1987, WANG Jinnian is one of the main researchers on hyperspectral remote sensing in early days in China, getting some innovative achievements on hyperspectral remote sensing information processing, modeling for spectral identification and its applications, such as:

1). Developed a series of algorithm on image processing and spectral analysis for Fine Infrared Multispectral Sensor (FIMS) imagery, especially identification technologies for geological alteration types which successfully extracted two golden alterations zone in Xinjiang Ebinur lake region;

2). Studied on airborne GERIS hyperspectral image to develop information analysis technology for “ image and spectra united as one” and quantitative identification model for single mineral spectrum which effectively had a detailed identification to stratum of Kalpin, Xinjiang based on 16nm spectral shift information between dolomite and carbonate caused by changes of Ca and Mg;

3). Developed and improved mineral spectral absorption index modeling which now is widely used on mapping and prospecting of mineral by hyperspectral remote sensing in China;

4). Developed and improved a software system the Hyperspectral Image Processing and Analysis System (HIPAS).
Acknowledgments

First of all, I would like to thank my supervisors, Professor Dr. Jean Sequeira, for his support, patience and friendship in all those years, also for being great examples of professionalism and seriousness in the research activity. I feel lucky and grateful to have the opportunity to work with them.

I would like to thank from the bottom of my heart to Prof. Qingxi Tong for his dedication and for his effort in improving my research and work experience. He guided my first steps on the exciting path of research in remote sensing, and supports me continually.

I would like to thank Dr. Xingfa Gu who was by my side all the time, encouraged me when I was on the right track and pushed me back on it every time when I was close to lose it.

I am sending all my gratitude and appreciation to Prof. Lifu Zhang and all of the other colleagues I do not mention here who definitely deserve my sincere acknowledgments, for their kindness, friendship and the good times we spent together.

Last but not least, I would like to thank my wife Jinfang Li, my daughter Hannah Wang and Ella Wang for supporting me all the time.
# Table of contents

Chapter 1 Introduction ................................................................. 1

1.1 Background of 3d hyperspetral geology mapping ...................... 1

1.2 Research significance .............................................................. 2

1.3 Research Status ................................................................. 3

1.3.1 Hyperspectral Remote Sensing Geology ........................... 3

1.3.2. Airborne Remote Sensing Geology ................................. 4

1.3.3. Field Mineral Spectral Analysis ................................. 5

1.3.4. Core Spectral Analysis .............................................. 6

1.3.5. 3D mineral mapping .............................................. 7

1.4 The report structure ........................................................... 7

Chapter 2 Mineral Mapping Theories and Hyperspectral data processing ............ 8

2.1 Mineral Spectral Theory ......................................................... 8

2.1.1 Electronic Processes ....................................................... 8

2.1.2 Vibrational Processes ................................................... 16

2.1.3 Mineral information quantitative extraction ...................... 32

2.2 Hyperspectral Data Processing .............................................. 38

2.2.1 Characteristics of Hyperspectral Data .............................. 38

2.2.2 Processing of Hyperspectral Data .................................... 40

2.2.3 Processing Systems of Hyperspectral Data at Home and Abroad .... 44

2.3 Mineral mapping ................................................................. 46

2.3.1 Concept of mineral mapping ........................................ 46

2.3.2 Processing of Mineral Exploration and Geological Assessment .... 46

2.3.3 Applications of mineral mapping ..................................... 47

Chapter 3 Hyperspectral data surface mineral mapping ............................ 57

3.1 Spectral Analysis Methods .................................................... 57

3.1.1 Field spectral data are spectral features analysis method ........... 57
3.1.2 Spectral Matching................................................................. 64
3.1.3 Spectral Unmixing............................................................... 65
3.1.4 Spectral classification .......................................................... 66
3.1.5 spectral feature extraction ................................................... 67
3.1.6 Endmember Extraction ....................................................... 68
3.2 Satellite images for Surface Mineralogy Mapping ................ 70
  3.2.1 Multi-spectral Images for Surface Mineralogy Mapping ....... 71
  3.2.2 hyperspectral Images for Surface Mineralogy Mapping ....... 73
3.3 Airborne hyperspectral images for Surface Mineralogy Mapping ...... 78
  3.3.1 Aviris ................................................................................. 78
  3.3.2 Hymap ............................................................................... 80
  3.4.3 CASI .................................................................................. 80
3.4 Field hyperspectral images for Surface Mineralogy Mapping .......... 82
  3.4.1 HySpex SWIR-320m ............................................................ 82
  3.4.2 PIMA ............................................................................... 84
3.5 Mineral mappings at the northern Death Valley ..................... 85
  3.5.1 Method ............................................................................. 85
  3.5.2 Mapping Results ................................................................. 88
  3.5.3 Discussion ....................................................................... 92
Chapter 4 Mapping drill cores using imaging spectrometry .......... 95
  4.1 The instrument of FISS ............................................................ 96
  4.2 Core drill imaging spectrometry system design ....................... 96
  4.3 Jiama 3D mapping ................................................................. 102
Chapter 5 Conclusions and Recommendation .......................... 103
  5.1 Conclusions ................................................................. 103
  5.2 Recommendation .............................................................. 106
References ............................................................................ 108
Chapter 1 Introduction

1.1 Background of hyperspectral 3D mineral mapping

With the rapid development of economy, the demand of mineral and resources is also growing fast. Mineral is an important foundation in developing economy and promoting society.

Due to the faraway locations of most of the key diggings, the current resource prospection has finished only 14% of basic investigations of 16 key metallogenic provinces, therefore, remote sensing is becoming a primary technology in direct mineralization information extraction and detailed geological survey, furthermore, the hyperspectral remote sensing will be the supporting technology in land resources survey and an important new technology in geological science and technology development in the new age[1].

The mineral are fundamental to all rocks and soils and is a key parameter to managing a sustainable Earth and mine exploration. The accurate 3D mineralogy mapping could understand better for the reactive transport processes of mineral systems, this will make it possible in generation of viable mineralization models for effective exploration, and will empower geoscientists with 3D mineral mapping capabilities to meet the challenges of sustainable exploration and mining, in particular, the recognition of new mineral deposits by suing spectral mineralogical vectors.

The Centre of Excellence for 3D Mineral Mapping (C3DMM, see: http://c3dmm.csiro.au ), sees a future in which the mining industry will routinely use 3D mineral maps derived by hyperspectral sensing to characterize prospective mineral systems with increased specificity and with reduced financial and environmental cost. The C3DMM is making efforts for a 2020 vision: a public, web accessible, measured, traceable, 3D mineral map of Australia based on drill core logging, airborne and satellite “geoscience tuned” data.

In China, there is also a “Spectral Crust” project to make 3D mineral mapping by using hyperspectral technology [2].

For 3D mineral mapping using hyperspectral remote sensing technology, there are five major challenges should be in making solutions in:

2. Surface Mineral Mapping Capabilities: to deliver a seamless surface mineral
map using current and future airborne and spaceborne hyperspectral systems

3. Information Systems: developing methods and algorithms to generate accurate measures of mineral information, and establish interfaces between different data formats, and research and build appropriate information access/delivery systems.

4. 3D Mineral Mapping: building 3D mineral models for mineral systems, improving knowledge about the formation, target vectors and exploitation of economic mineral deposits.

1.2 Research significance

Imaging spectroscopy can be applied to identify surface mineralogy based upon distinguishing absorption features in the spectral response from exposed materials. Depending upon the surface material, electronic and vibrational processes can preferentially absorb energy as a function of wavelength, creating characteristic absorption features for both organic and inorganic materials. The characteristic absorption features, located within the visible to shortwave-infrared range of ~0.4–2.5 μm, can be used individually or in combination to identify and map surface mineralogy. It made more difficult for mineral identification by the presence of naturally-occurring geologic mixtures, such as coatings or intimate mixtures, and differing grain sizes which affect the spectral response, depending upon the wavelength. This energy response across wavelengths depends on the nature of the material with which energy interacts, both chemically and structurally. Even with these complications, the atomic or molecular level of the energy–material interaction provides a specific diagnostic tool for mapping mineralogy that can be effectively utilized on a micro to macro spatial scale.

The imaging spectroscopy provides an important tool in answering this question by providing a means for mapping the aerial extent of mineral associations [3]. Absorption feature descriptions, such as depth, width, and asymmetry can be applied to characterize spectra with respect to known sample materials.

Traditionally, geology deals with the composition, structure, and history of the Earth. However, more and more geology deals with processes that have formed the Earth and other planets indicating that geology becomes more multidisciplinary and more positioned on issues of societal relevance. Geological remote sensing has been defined in many literatures, the remote sensing data, which can be field based, airborne or space-borne geophysical measurements, have been applied to study geology widely. Most of the geologic remote sensing in the visible-near infrared (VNIR), shortwave infrared (SWIR), mid infrared (MIR) and thermal infrared (TIR) part of the spectrum resulted from pioneering work of Hunt and Salisbury who meticulously measured mineral and rock spectra forming the basis for airborne and spaceborne instruments. Remote sensing geologists have actively contributed to the
development of active sensor technology (predominantly SAR and InSAR) and passive sensor technology (multispectral and hyperspectral remote sensing in the VNIR to SWIR and TIR parts of the spectrum).

1.3 Research Status

1.3.1 Hyperspectral Remote Sensing Geology

For many years, the primary sources of remote sensing data come from monochromatic and multispectral sensors that generate images either at a fixed wavelength or at several specific and discrete spectral bands. Data and images produced from satellite-based or airborne multispectral imaging systems, such as the 4-band MSS (multispectral scanner) and 7-band TM (Thematic Mapper) Landsat data, and the 3-band SPOT images, have made up the majority of remote sensing data for decades. Typically, the bandwidth of these types of sensors is broad (usually greater than 0.07μm). Hyperspectral data, on the other hand, are data collected at a higher spectral resolution (narrower bandwidth, typically 0.02μm or less) and with contiguous spectral bands.

The first satellite imaging spectrometer was the LEWIS Hyperspectral Imager (HSI) from TRW Company, which was launched in 1997 but failed.

The European Space Agency currently operates the Compact High Resolution Imaging Spectrometer, CHRIS [4-6], on board the Proba-1 (9 years of operation) which measures directional spectral reflectance using multiple viewing and illumination geometries, with a spectral range of 0.415–1.050μm, a spectral resolution of 5–12 nm up to 19 spectral bands and a spatial resolution of 20 m at nadir on a 14 km swath.

The Advanced Space borne Thermal Emission and Reflection Radiometer (ASTER) was launched in 1999. ASTER is a multispectral scanner that orbits ~ 705 km above the Earth [7-9]. An ASTER scene typically covers an area of 60 km by 60 km. There are 14 individual bands that cover the VNIR, SWIR, and TIR regions of the EM field. There are 3 bands in the VNIR, 6 over the SWIR, and 5 in the TIR. The 3 bands in the VNIR have a spatial resolution of 15 meters, while those in the SWIR have 30 meter, and finally those in the TIR have 90 meters resolution.

Satellite-based hyperspectral imaging became a reality in November 2000 with the successful launch and operation of the Hyperion instrument aboard the EO-1 satellite [10-12]. Within the framework of the New Millennium Program NASA launched Hyperion on New Millennium Program (NMP) Earth Observing (EO)-1, the Hyperion, which based on the LEWIS HSI concept, has 220 spectral bands (from 0.4 to 2.5μm) with a 30 m spatial resolution imaging a 7.5 km by 180 km area per frame,
flying on a 705 km circular sun-synchronous orbit at a 98.7° inclination which allows to match within one minute the Landsat 7 orbit.

SEBASS is a hyperspectral sensor with 128 bands covering the spectral range of 3.0-5.5 μm and 7.8-13.5 μm, with a ~1.0° instantaneous field of view and ~2 – 5 m spatial resolution[13, 14].

### 1.3.2. Airborne Remote Sensing Geology

The first scanning imaging spectrometer was the Scanning Imaging Spectroradiometer (SIS) constructed in the early 1970s for NASA’s Johnson Space Centre. After that, civilian airborne spectrometer data were collected in 1981 using a one-dimensional profile spectrometer developed by the Geophysical Environmental Research Company, which acquired data in 576 channels covering the 0.4–2.5 m wavelength followed by the Shuttle Multispectral Infrared Radiometer (SMIRR) in 1981. The first imaging device was the Fluorescence Line Imager (FLI) developed by Canada’s Department of Fisheries and Oceans in 1981. NASA’s Jet Propulsion Laboratory developed the Airborne Imaging Spectrometer (AIS) of which the first version became operational in 1983 (128 spectral bands, 1.2–2.4 m, 32 pixels across-track for AIS-1 and 64 for AES-2). Since 1987, NASA operates the Airborne Visible/Infrared Imaging Spectrometer [15-17], AVIRIS (224 bands, 0.4 to 2.5 m region, sampling interval and resolution <10 nm, FOV 30°, 614 pixel swath).

Several companies developed hyperspectral sensors. The Finnish Spectral Imaging (SPECIM) manufactures the AISA (Airborne Imaging Spectrometer for Applications) with the family of Airborne Imaging Spectrometers (the AisaEAGLE, VNIR 0.400–0.970 m, 512 or 1024 spatial pixels, 488 spectral bands; AisaHAWK, SWIR 0.970–2.500 m, 320 spatial pixels, 254 spectral bands; AisaOWL, 8–12 m, 384 pixels, 84 spectral bands). In Canada, ITRES developed the Compact Airborne Spectrographic Imager (CASI), operational since 1989 (288 spectral channel, 1.9 nm. resolution, 512–1500 pixels across track, 400–1100 range) and similar systems in the SWIR (SASI), MIR (MASI) and TIR (TASI). The Geophysical Environmental Research Corporation (GER) developed the GER Imaging Spectrometer (GERIS), the Digital Airborne Imaging Spectrometer (DAIS; 72 channels, 0.4–2.5 m, FOV of 3.3 mrad and six channels in the 8–12 m region). The Australia-based company Integrated Spectronics designed the Hyperspectral Mapper (HyMap; in the U.S. known as Probe-1) a 126 channel sensor covering the 0.4–2.5 m region.

The Airborne Visible/Infrared Imaging Spectrometer (AVIRIS), with flights beginning in 1987, is one of the earliest airborne hyperspectral scanners to be used for geologic applications [16, 18]. AVIRIS consists of 224 contiguous bands that cover much of the VNIR and SWIR, from 0.60 – 2.50 microns. Due to the contiguous design of the AVIRIS bands, it is possible to resolve subtle, and unique, absorption features to specific mineral species. AVIRIS has a nominal spectral resolution of ~ 10 nm. A
spatial resolution of either 4 or 20 m can be achieved by varying the altitude at which the craft is flown.

A wide variety of VNIR and SWIR airborne imaging spectrometers have been or are currently being flown. The ProSpecTIR-VS hyperspectral system operated by SpecTIR, LLC (www.spectir.com), is a custom-integrated system that incorporates Specim’s (www.specim.fi) Airborne Imaging Spectrometer for Applications (AISA), Eagle (VNIR) and Hawk (SWIR) imaging spectrometers. The combination of these two high-performance sensors provides for the simultaneous acquisition of full hyperspectral data covering the 0.4–2.45 μm spectral range. The two imaging spectrometers are co-aligned and generate a single, full-spectrum data cube covering 320 pixels cross-track. In airborne operation, as a push-broom instrument and utilizing a 24° scan and 0.075° (approximately 1.3 m rad) instantaneous field of view (IFOV), the system achieves spatial resolutions varying from 0.5 to 5 m depending upon altitude and platform speed.

HyMap is an aerially-mounted hyperspectral sensor with 126 bands covering the visible, near-infrared, and shortwave-infrared wavelength range (VNIR/SWIR) from 0.45 to 2.5 μm, with sampling intervals or bandwidths of 15–20 nm[19-21]. HyMap’s instantaneous field of view is ~2.0° and its spatial resolution, which is dependent upon the height at which the sensor is flown, is ~3–5 m. Its spectral and spatial resolution in conjunction with its high signal to noise ratio (greater than 500:1) allows HyMap to record diagnostic absorption features which can be used to effectively distinguish surface mineralogy.

1.3.3. Field Mineral Spectral Analysis

With the development of very compact and sophisticated spectrometers and spectroradiometers, field spectroscopy is evolving as a robust technique in mineral exploration and geological mapping. Field spectroscopy also plays a key role for scaling-up of energy–matter interactions from field scale of a few centimeters to satellite pixel scale of a few meters. However, understanding on various influence parameters such as source-sensor geometry, grain size, instrument calibration, spectral acquisition procedure, scheme of library spectral candidate selection and the appropriateness of un-mixing procedure is vital for effective utilization of this technique.

Ground-based imaging spectrometers have some limitations in mineral identification studies compared to airborne and spaceborne remote sensing surveys. The differences in scale and spatial extent between these distinct modes of observation often preclude the former due to the increased time or cost involved for an effectively smaller surface area of measurement. Instead, discrete field-based in-situ radiometric measurements and ancillary analyses are commonly used for comparison and corroboration of air- or space-borne remotely sensed
measurements. However, limitations imposed upon traditional remote sensing data in terms of the spatial, spectral and radiometric resolution suggest that ground-based image data may have utility when high spatial resolution is required for particular geologic applications.

Spectral measurements of field samples were taken in the lab using a portable field spectrometer, the FieldSpec 3 Analytical Spectral Device (ASD). The ASD’s wavelength sampling ranges from 3 to 10 nm, over a spectral range of 0.350 – 2.500 μm. A contact probe with a 1 cm diameter spot size and its own illumination was used to collect the spectral measurements.

The field sample spectra were examined both manually and with an algorithm provided in the ENVI software, in order to select spectra that best represent the spectral classes of materials present in the samples. An “image cube” of spectral measurements from the field samples was created in order to facilitate the examination of the field sample spectra. The image cube displays each measurement as a pixel with associated spectral data, just as would be seen in a satellite or aerially-acquired image, however without the neighboring spatial coherency that would be expected in an image acquired of land surfaces. Creating an image cube allowed the data to be brought into ENVI. Field sample spectral data were classified by manual inspection of each spectrum and application of the Spectral Feature Fitting (SFF) algorithm, which allowed a systematic classification of the sample spectra. SFF is a classification method compares the shape of the endmember spectrum to the pixel spectra after the spectra have been continuum-removed in order to normalize the spectral data.

1.3.4. Core Spectral Analysis

In addition to typical airborne and satellite hyperspectral data acquisitions, spectroscopy has also been used in a limited way for analysis of drill cores and for outcrop scanning. More recently, efforts have been directed at operational spectral logging of drill cores using automated methods. Core imaging efforts are, however, still in the early stages of development. The research described here brings these airborne, core and outcrop imaging modalities together to demonstrate an integrated approach to mineral mapping for mine site exploration, evaluation and development.

The ProSpecTIR-VS sensor was operated in three different modes for the purposes of this research: (1) airborne overflight data at approximately 1 m spatial resolution, (2) core and rock-chip scans using a custom scanning bed and artificial (halogen) illumination at approximately 2 mm spatial resolution and (3) mine-wall scans using a truck-mounted scanning configuration and solar illumination at approximately 4 cm spatial resolution.
In January 2005, Blue Mine diamond drill core was scanned by the CSIRO core scanning HyLogger system at PIRSA’s Glenside Core Library. The HyLogger has three instruments installed on a support frame: a hyperspectral spectroradiometer (450–2500 nm); a three band, high resolution line scan camera; and a laser profilometer. The core scanner provides a rapid means of gathering semi-quantitative statistical distributions of minerals down hole. When linked with assay data, this provides a powerful tool for understanding drilling results in the context of deposit.

1.3.5. 3D mineral mapping

To solve the problem that the amount of global mineral resources is decreasing rapidly, Dr. Cars came up with the notion of “a glass earth” which aims at uncovering a kilometer underground in Australia and the geological processes happen there in order to find out the next generation mega-deposits in Australia[22-25]. As a similar program, the Minerals Down Under consists of 3 subprojects: ROES, Hyperspectral Logging, and Enabling Geoscientific Data Interoperability. ROES is a new hard-rock underground mining method to drill, blast and recover ore using unmanned machines. Hyperspectral Logging provides logging and analysis software of drill core, drill chips and blast hole cuttings without subjectivity. Geoscientific Data Interoperability is supporting to break the barrier of poor geospatial data interchange. This program promotes the development of geological mineral resources detection in Australia.

The Chang'e Moon Project drives development of a series of space detecting technology such as satellite, sensor, rocket launching and navigation and location in China [26-28]. In the aspect of mineral resources detection, our country has made a giant progress and has gathered a lot of experience in hyperspectral load research, hyperspectral mineral detection technology and hyperspectral data processing, however, these technologies have not been organic integrated yet. I and my team have made a proposal of “Spectral Crust” project to make 3D mineral mapping by using hyperspectral technology integrated satellite, airborne, ground and drill hyperspectral data.

1.4 The report structure

This report will include 5 chapters totally: the first chapter is Introduction, which has been stated above; the second chapter will introduce mineral mapping theories and hyperspectral data processing; the third chapter will be hyperspectral data surface mineral mapping, which is consisted of satellite, airborne and field hyperspectral data processing; the fourth chapter will be mapping of drill cores using imaging spectrometry, in which our self-made imaging spectrometer will be introduced; the fifth chapter is conclusions and recommendation.
Chapter 2 Mineral Mapping Theories and Hyperspectral Data Processing

2.1 Mineral Spectral Theory

Using hyperspectral remote sensing technology, an extensive range of mineral can be remotely mapped, including: iron oxides, clays, micas, chlorites, amphiboles, talc, serpentines, carbonates, quartz, garnets, pyroxenes, feldspars and sulphates, as well as their physicochemistries such as cation composition and long and short range order.

Geological remote sensing is performed through atmospheric windows where electromagnetic radiation (EMR) is allowed to pass without significant attenuation. The five atmospheric windows available for remote mineral mapping include the visible to near infrared (VNIR), the shortwave infrared (SWIR), the mid-infrared (MIR), the thermal infrared (TIR) and the microwave wavelength regions (Figure 2.1). The ultraviolet (UV) and far infrared (FIR) wavelength regions are not available.

![Atmospheric transmission spectrum.](image)

What causes absorption bands in the spectra of minerals? There are two general processes: electronic and vibrational. Burns examines the details of electronic processes, and Farmer covers vibrational. These two books are significant works providing the fundamentals as well as practical information. A shorter introduction to the causes of absorption bands in minerals is given by Hunt and Gaffey for the visible and near-infrared.

2.1.1 Electronic Processes

Isolated atoms and ions have discrete energy states. Absorption of photons of a specific wavelength causes a change from one energy state to a higher one. Emission
of a photon occurs as a result of a change in an energy state to a lower one. When a photon is absorbed it is usually not emitted at the same wavelength[29]. For example, it can cause heating of the material, resulting in grey-body emission at longer wavelengths.

In a solid, electrons may be shared between individual atoms. The energy level of shared electrons may become smeared over a range of values called "energy bands." However, bound electrons will still have quantized energy states[30, 31].

(1) Crystal Field Effects.

The most common electronic process revealed in the spectra of minerals is due to unfilled electron shells of transition elements (Ni, Cr, Co, Fe, etc.). Iron is the most common transition element in minerals. For all transition elements, d orbitals have identical energies in an isolated ion, but the energy levels split when the atom is located in a crystal field. This splitting of the orbital energy states enables an electron to be moved from a lower level into a higher one by absorption of a photon having an energy matching the energy difference between the states [32]. The energy levels are determined by the valence state of the atom (e.g. Fe2+, Fe3+), its coordination number, and the symmetry of the site it occupies. The levels are also influenced by the type of ligands formed, the extent of distortion of the site, and the value of the metal-ligand interatomic distance. The crystal field varies with crystal structure from mineral to mineral, thus the amount of splitting varies and the same ion (like Fe2+) produces obviously different absorptions, making specific mineral identification possible from spectroscopy (Figure 2.2-2.6).
Figure 2.3: VNIR spectra of iron-oxide bearing minerals vs. other major rock forming minerals

Figure 2.4a: Reflectance spectra of two olivines showing the change in band position and shape with composition. The 1-µm absorption band is due to crystal field absorption of Fe$^{2+}$. "Fo" stands for forsterite (Mg$_2$SiO$_4$) in the forsterite-fayalite (Fe$_2^{2+}$SiO$_4$) olivine solid solution series. The Fo 29 sample (K13291 from King and Ridley) has a FeO content of 53.65%, while the Fo 91 sample (GDS 71; labeled Twin Sisters Peak in King and Ridley) has a FeO content of 7.93%. The mean grain size is 30 and 25 µm respectively. The 1-µm band position varies from about 1.08 µm at Fo 10 to 1.05 µm at Fo 90 (King and Ridley).
Figure 2.4b. Same as for Figure 2.4a but for mid-infrared wavelengths. Note the shifts in the spectral features due to the change in composition.

Figure 2.5a. Reflectance spectra of two pyroxenes showing the change in Fe$^{2+}$-absorption band position and shape with composition (from Clark). Diopside, sample NMNH18685, is CaMgSi$_2$O$_6$ but some Fe$^{2+}$ substitutes for Mg. Bronzite, sample HS9.3B, is (Mg,Fe)SiO$_3$ with mostly Mg. The 1-µm versus the 2-µm band position of a pyroxene describes the pyroxene composition, Figure 2.5c. The diopside spectrum is offset 0.2 units upward.
Figure 2.5b. Same as for Figure 2.6a, but for mid-infrared wavelengths. Note the shifts in the spectral features due to the change in composition.

Figure 2.5c. Pyroxene 1-µm versus 2-µm absorption band position as a function of composition, as adapted from Adams by Cloutis and Gaffey[33][22]. Open circles have > 11% wollastonite (Wo), and solid symbols < 11 % Wo. Samples with zoned or evolved phases are marked by "Z." Other samples not following the "normal" trend include those with >1% TiO$_2$ (Ti), > 1% Cr$_2$O$_3$ (Cr), or >4% Al$_2$O$_3$. 
Figure 2.6a. Reflectance spectra of the iron oxide hematite ($\text{Fe}_2\text{O}_3$) and iron hydroxide goethite (FeOOH, from Clark). The intense charge-transfer band in the UV (< 0.4 µm) is “saturated” in reflectance, so only first surface (specular) reflection is seen in these spectra. The 0.9-µm and 0.86-µm absorption features are due to Laporte-forbidden transitions (e.g. Morris et al; Sherman[34][23] and references therein). The absorption at 2.7-3 µm is due to trace water in the samples and in the case of goethite, the OH. The goethite spectrum is offset upward 0.2 units.

Example Fe2+ absorptions are shown in Figure 2.4a (olivines), and Figure 2.5a (pyroxenes). Note the shift in band position and shape between the different compositions. Example Fe3+ absorptions are shown in goethite (FeOOH) and hematite (Fe2O3) in Figure 2.6a. Compositional changes also shift vibrational absorptions, discussed below, and as seen in Figures 2, 4b, 2.5b, and 2.6b. The compositional shifts of the electronic absorptions have been studied by Adams and Cloutis and Gaffey for pyroxenes and are shown in Figure 2.5c and by King and Ridley for olivine.
The unfilled shells of rare earth ions involve deep-lying electrons, which are well shielded from surrounding crystal fields so the energy levels remain largely unchanged. Thus, absorption bands due to rare earth elements are not diagnostic of mineralogy but to the presence of the ions in the mineral (Figure 2.7).

**Figure 2.7a.** Reflectance spectra of rare-earth oxides. These absorptions are due to crystal-field transitions involving deep-lying electrons of the rare-earth element and do not shift when the rare-earth ion is in another mineral. Each spectrum is offset by 1.0 unit for clarity. Spectra from Clark et al.

**Figure 2.7b.** Same as Figure 2.7a, except showing absorptions in the visible region. Spectra are offset 1.0 unit for clarity. Spectral resolution is about 1 nm, critically sampled.

(2) Charge Transfer Absorptions

Absorption bands can also be caused by charge transfers, or by inter-element transitions where the absorption of a photon causes an electron to move between ions or between ions and ligands. The transition can also occur between the same
metal in different valence states, such as between Fe\(^{2+}\) and Fe\(^{3+}\)[35]. In general, absorption bands caused by charge transfers are diagnostic of mineralogy. Their strengths are typically hundreds to thousands of times stronger than crystal field transitions. The band centers usually occur in the ultraviolet with the wings of the absorption extending into the visible. Charge transfer absorptions are the main cause of the red color of iron oxides and hydroxides (Figure 2.7a). Morris et al. studied the details of sub-micron iron oxides where it was found that the absorption bands rapidly decrease in intensity. This occurs because of the increased surface to volume ratio at small grain size results in a greater proportion of grain boundaries where crystal field effects are different, resulting in lower magnetic coupling and reduced absorption strength. Other iron oxides probably show similar effects. Reflectance spectra of iron oxides have such strong absorption bands that the shape changes significantly with grain size. Small shifts in absorption band position are also observed due to substitution of other elements, like aluminum for iron in hematite (e.g. Morris et al.) and references therein) but more work needs to be done to fully understand the effects.

(3) Conduction Bands

In some minerals, there are two energy levels in which electrons may reside: a higher level called the "conduction band," where electrons move freely throughout the lattice, and a lower energy region called the "valence band," where electrons are attached to individual atoms. The difference between the energy levels is called the band gap. The band gap is typically small or non-existent in metals, and very large in dielectrics. In semiconductors, the band gap corresponds to the energy of visible to near-infrared wavelength photons and the spectrum in these cases is approximately a step function. The yellow color of sulfur is caused by such a band gap. The minerals cinnabar (HgS) and Sulfur (S) have spectra showing the band gap in the visible (Figure 2.8).

Figure 2.8. Reflectance spectra of Sulfur, S, (top) and cinnabar, HgS, (bottom) showing conduction bands in the visible (from Clark et al).
(4) Color Centers

A few minerals show color due to absorption by "color centers." A color center is caused by irradiation (e.g. by solar UV radiation) of an imperfect crystal. Crystals in nature have lattice defects that disturb the periodicity of the crystal [36]. For example, defects might be caused by impurities. These defects can produce discrete energy levels and electrons can become bound to them. The movement of an electron into the defect requires photon energy. The yellow, purple and blue colors of fluorite are caused by color centers.

2.1.2 Vibrational Processes

The bonds in a molecule or crystal lattice are like springs with attached weights: the whole system can vibrate. The frequency of vibration depends on the strength of each spring (the bond in a molecule) and their masses (the mass of each element in a molecule). For a molecule with N atoms, there are 3N-6 normal modes of vibrations called fundamentals. Each vibration can also occur at roughly multiples of the original fundamental frequency. The additional vibrations are called overtones when they involve multiples of a single fundamental mode, and combinations when they involve different modes of vibrations.

A vibrational absorption will be seen in the infrared spectrum only if the molecule responsible shows a dipole moment (it is said to be infrared active). A symmetric molecule, like N2 is not normally infrared active unless it is distorted (for example, when under high pressure). Vibrations from two or more modes can occur at the same frequency, and because they can't be distinguished, are said to be degenerate. An isolated molecule with degenerate modes may show the modes at slightly different frequencies in a crystal because of the non-symmetric influences of the crystal field.

A free molecule can rotate and move translational, but even in a solid partial rotation and slight translation can occur. These motions are called lattice modes and typically occur at very low energies (longer mid-infrared wavelengths), beyond about 20 µm.

Traditionally, the frequencies of fundamental vibrations are labeled with the letter nu (ν) and a subscript (Herzberg). If a molecule has vibration fundamentals ν₁, ν₂, ν₃, then it can have overtones at approximately 2ν₁, 3ν₁, 2ν₂ and combinations at approximately ν₁+ν₂, ν₂+ν₃, ν₁+ν₂+ν₃, and so on. These examples used summations of modes, but subtractions are also possible (e.g. ν₁+ν₃−ν₂). Each higher overtone or combination is typically 30 to 100 times weaker than the last. Consequently, the spectrum of a mineral can be quite complex. In reflectance spectroscopy, these weak absorptions can be measured easily and diagnostic
information routinely gained from 2nd and 3rd overtones and combinations (e.g. Figures 2.4b, 2.5b, 2.6b, 2.9, 2.10, and 2.11).

Figure 2.9a. Reflectance spectra of calcite, dolomite, beryl, gypsum, alunite, rectorite, and jarosite showing vibrational bands due to OH, CO$_3$ and H$_2$O, from Clark et al.
Figure 2.9b. Reflectance spectra of phlogopite, biotite, pyrophyllite, muscovite, epidote, and illite showing vibrational bands due to OH and H$_2$O, from Clark et al.

Figure 2.9c. Reflectance spectra of hectorite, halloysite, kaolinite, chrysotile, lizardite, and antigorite showing vibrational bands due to OH (from Clark et al).
Figure 2.9d. Subtle spectral differences in the kaolinite group minerals near 2.2-µm. Kaolinite CM9 is well crystallized (WXL) while KGa-2 is poorly crystallized (PXL). Spectral bandwidth is 1.9 nm and sampling is 0.95 nm. Each spectrum was scaled to 0.7 at 2.1 µm then offset up or down so that the curves to not overlap. Original reflectance was between 0.5 and 0.8.

Figure 2.10. Comparison of calcite (CaCO$_3$) and dolomite (CaMg(CO$_3$)$_2$) spectra in the mid-infrared showing small band shifts due to the change in composition between the two minerals. The level change (calcite higher in reflectance than dolomite) is because the calcite has a smaller grain size. The numbers indicate the fundamental stretching positions of $\nu_1$, $\nu_2$, $\nu_3$, and $\nu_4$. The $\nu_2$ stretch is infrared inactive, but may be weakly present in carbonates. The $\nu_3$ fundamental is so strong, only a reflection peak is seen in these spectra.
Figure 2.11. Mid-IR spectra of gypsum, CaSO$_4$2H$_2$O. (Top) and montmorillonite, (Al, Mg)$_8$[(Si$_4$O$_{10}$)(OH)$_2$]$10$H$_2$O (bottom). The gypsum curve is offset upward 1.0 unit for clarity. Both samples have very low reflectance because of the water content of the samples. Water is a strong infrared absorber. The montmorillonite also has a small grain size, which also tends to produce low mid-infrared reflectance because of the strong absorption in the mid-infrared.

Figure 2.12a. Spectral signature diagram (from Hunt[36][25]). The widths of the black bars indicate the relative widths of absorption bands.
Lattice modes are sometimes denoted by $\nu_T$ and $\nu_R$ and also coupled with other fundamentals, resulting in finer structure seen in some spectra. The causes of vibrational absorptions in mid-IR spectra are summarized in Figure 2.12b from Hunt.

Mid-infrared reflectance spectra of quartz are shown in Figure 2.13. The strong 9-µm Si-O-Si asymmetric stretch fundamental is obvious from the reflection maximum. The O-Si-O bending mode occurs near 25 µm and is the second strongest absorption. The absorption between 12 and 13 µm is the Si-O-Si symmetric stretch fundamental.

Olivine spectra in the mid-infrared are shown in Figure 2.4b. When Mg is present, a strong absorption appears near 23 µm, perhaps seen in the Fo 91 spectrum. The Si-O-Si asymmetric stretch fundamental occurs near 11 µm, and a weaker symmetric absorption occurs near 12 µm. The absorptions shift with composition as shown in Figure 2.4b, and discussed in more detail in Farmer.

Pyroxene mid-infrared spectra are shown in Figure 2.5b. The Si-O fundamentals are at similar to other silicates, as indicated in Figure 2.12b.
Iron oxide and iron hydroxide mid-infrared spectra are shown in Figure 2.6b. Because iron is more massive than silicon, Fe-O fundamentals will be at longer wavelengths than Si-O stretching modes. Hematite, Fe₂O₃, has 3 strong stretching modes between 16 and 30 µm. Because iron oxides and hydroxides tend to be fine grained, typically less than the wavelength of mid-infrared photons, and because of the strong absorption in the mid-infrared, iron oxides tend to be dark in reflectance showing few features beyond about 12 µm. The hematite in Figure 2.6b has a small amount of water as evidenced by the 3-µm absorption, and a moderate amount of organics as seen by the C-H stretch fundamental near 3.4 µm. The goethite, FeOOH, having hydroxyl has strong 3-µm absorption. The olivines (Figure 2.4) and pyroxenes (Figure 2.5) also show small amounts of water in the sample as seen by the 3-µm absorptions in their spectra.

(1) Water and Hydroxyl

Water and OH (hydroxyl) produce particularly diagnostic absorptions in minerals. The water molecule (H₂O) has N=3, so there are 3N-6=3 fundamental vibrations. In the isolated molecule (vapor phase) they occur at 2.738 um (ν₁, symmetric OH stretch), 6.270 um (ν₂, H-O-H bend), and 2.663 um (ν₃, asymmetric OH stretch). In liquid water, the frequencies shift due to hydrogen bonding ν₁=3.106 um, ν₂=6.079 um, and ν₃=2.903 um.

The overtones of water are seen in reflectance spectra of H₂O-bearing minerals (Figure 2.9). The first overtones of the OH stretches occur at about 1.4 um and the combination of the H-O bend with the OH stretches is found near 1.9 um. Thus, a mineral whose spectrum has a 1.9-um absorption band contains water (e.g. Hectonite and halloysite in Figure 2.9c), but a spectrum that has a 1.4 um band but no 1.9-um band indicates that only hydroxyl is present (e.g. Kaolinite in Figure 2.9c has only a small amount of water because of the weak 1.9-um absorption but a large amount of OH). The hydroxyl ion has only one mode and its wavelength position is dependent on the ion to which it is attached. In spectra of OH-bearing minerals, the absorption is typically near 2.7 to 2.8 um, but can occur anywhere in the range from about 2.67 um to 3.45 um (e.g. See Clark et al. and reference therein). The OH commonly occurs in multiple crystallographic sites of a mineral and is typically attached to metal ions. Thus, there may be more than one OH feature. The metal-OH bend occurs near 10 um (usually superimposed on the stronger Si-O fundamental in silicates). The combination metal -OH bend plus OH stretch occurs near 2.2 to 2.3 um and is very diagnostic of mineralogy (e.g. See Clark et al. and reference therein).
(2) Carbonates

Carbonates also show diagnostic vibrational absorption bands (Figure 2.9a, 2.10). The observed absorptions are due to the planar CO$_3^{2-}$ ion. There are four vibrational modes in the free CO$_3^{2-}$ ion: the symmetric stretch, $\nu_1$: 1063 cm$^{-1}$ (9.407 um); the out-of-plane bend, $\nu_2$: 879 cm$^{-1}$ (11.4 um); the asymmetric stretch, $\nu_3$: 1415 cm$^{-1}$ (7.067 um); and the in-plane bend, $\nu_4$: 680 cm$^{-1}$ (14.7 um). The $\nu_1$ band is not infrared active in minerals. There are actually six modes in the CO$_3^{2-}$ ion, but 2 are degenerate with the $\nu_3$ and $\nu_4$ modes. In carbonate minerals, the $\nu_3$ and $\nu_4$ bands often appear as a doublet. The doubling has been explained in terms of the lifting of the degeneracy (e.g. See White) due to mineral structure and anion site.

Combination and overtone bands of the CO$_3^{2-}$ fundamentals occur in the near IR. The two strongest bands are $\nu_1+2\nu_3$ at 2.50-2.55 um (4000-3900 cm$^{-1}$), and $3\nu_3$ at 2.30-3.35 um (4350-4250 cm$^{-1}$; e.g. Figure 2.9a). Three weaker bands occur near 2.12-2.16 um ($\nu_1+2\nu_2+\nu_4$ or $3\nu_1+2\nu_2$; 1720-1630 cm$^{-1}$), 1.97-2.00 um ($2\nu_1+2\nu_3$; 4570-4470 cm$^{-1}$), and 1.80-1.84 um ($3\nu_1+3\nu_2$; 4760-4660 cm$^{-1}$).
5080-5000 cm$^{-1}$, and 1.85-1.87 um ($\nu_1+3\nu_3$; 5400-2350 cm$^{-1}$ e.g. Figure 2.9a) (e.g. Hunt and Salisbury). The band positions in carbonate vary with composition. An example of such a band shift is seen in Figure 2.9a, 2.10.

(3) Other minerals

a. White Mica Chemistry

Infrared spectral reflectance measurements of white micas made in the field, underground or on drill – whole material, can be used to map compositional variations that may change spatially with proximity to ore and with host lithologies.

The white micas are sheet silicates consisting of layer of octahedrally coordinated ions sandwiched between linked Si/Al tetrahedral with large 12-fold coordinated cations between the tetrahedral sheets (Deer, Howie and Zussman; Figure 2.16).

They have a general formula-
\[ X_2Y_2Z_8O_{20}(OH)_4 \]
where  
- $X$=large cations in 12 – fold coordination (e.g. K$^+$)
- $Y$=octahedrally coordinated cations e.g. Al$^{3+}$
- And $Z$=tetrahedrally coordinated cations e.g. Si$^{4+}$ and Al$^{3+}$.  
(OH) sites may also be occupied by halogen anions, particularly F$^-$ and Cl$^-$

The spectra of these micas appear to show differences that are related to compositions at 1400, 2200, 2350 and 2450 nm (Figure 2.17), with the 2200 nm feature most useful, due to the great variation in wavelengths in that region.
Figure 2.17. Spectra for paragonite, muscovite, phengite and illite

Figure 2.18. Spectra for paragonite, muscovite and phengite in the 1400 nm region.

Figure 2.19. Spectra for paragonite, muscovite and phengite in the 2000-2500 nm regions.
The wavelength of the 2200 nm feature for white micas varies inversely with the amount of trivalent cations in octahedral coordination within the mica structure. Thus paragonite (being Al-rich) has shorter wavelengths and phengite (being Al-poor) longer wavelengths than muscovite itself. Because the species of trivalent ion is not important for this relationship, it is not possible to spectrally predict a priori which trivalent ions are present in mica, i.e. Fe$^{3+}$, Cr$^{3+}$ and V$^{3+}$ substitution in micas cannot be distinguished spectrally. Unfortunately, this means that the Fe: Mg ratios (which have often proven useful in hydrothermal alternation studies) cannot be predicted spectrally from the wavelength of the main 2200 nm absorption feature. The potential to gain compositional information by more detailed deconvolution of the longer wavelength tail of the absorption feature has not however been fully tested. Furthermore, because phengitic micas tend to form in ferromagnesian-rich environments and such mica is more stable to weathering than biotite or chlorite, the former presence of chlorite/biotite may sometimes be inferred in phengite-bearing regolith samples.

Although the substitution of Na for K relates to the shortening of the wavelength of the 2200 nm feature in micas, the association is actually due to the increasing Al in octahedral coordination in paragonitic micas.

Because illite has the same octahedral structure as muscovite, illite shows a similar spectral response to the white micas, except for the stronger development of the 1900 nm water feature. Thus differentiation of illite from muscovite may be difficult, especially in regolith samples where other hydrated phases (e.g. smectites) make a substantial contribution to the intensity of the 1900 nm feature. Halogens (especially F) tend to result in strong hydrogen bonding and the development of an “anomalous water” feature at 1940 nm. Although this cannot be specifically related to halogen in mica, the association of high halogen contents in micas with high contents in other minerals suggests that the presence of “anomalous water” may represent a guide to halogen in mica, which may in turn imply a significant Mg content in the mica in most cases.
b. Feldspars

The feldspars are a ubiquitous mineral group in the Earth’s crust. There are 11 major types of feldspar minerals each showing different structure and chemistry, the precise nature of which is related to the environment of their crystallization. As a consequence, feldspar mineralogy is useful in the classification of many rocks, especially igneous rocks. Most feldspar can be considered as part of a ternary system (Figure 2.21) with the three apices of this diagram defined by Na$_2$Si$_3$O$_8$, K$_2$Si$_3$O$_8$, and CaSi$_3$O$_8$. Members of the series between the Na and K endmembers are considered alkali feldspars (microcline, orthoclase, sanidine, anorthoclase) and those between Na and Ca are considered plagioclase feldspars (with increasing Ca the series comprises albite, oligoclase, andesine, labradorite, bytownite and anorthite). The alkali feldspars can contain up to 10% Ca in solid solution whereas the plagioclase can contain up to 10% K.

The mineralogy of the K endmember depends on the temperature of formation and hence structure of the feldspar. The alkali feldspar that forms at the highest temperatures of crystallisation is sanidine, which is monoclinic. Orthoclase, which is also monoclinic, forms at moderate temperatures, while microcline, which is triclinic, forms at the lowest temperatures. Adularia is a low temperature, K-rich (Or$_{90}$Ab$_{5}$An$_{1}$) feldspar with variable structure and confined to Alpine vein-type paragenesis (Deer et al.). A more complex relationship with temperature is found for the plagioclase feldspars with both monoclinic and triclinic forms possible for all solid solution chemistries.

Figure 2.20. White Mica Chemistry
Various workers have measured the TIR spectral properties of feldspar minerals. They have shown that the alkali-feldspar minerals and plagioclase feldspars have diagnostic spectral behavior, especially in the 8 to 11 μm wavelength region where there exist changes in the number and position of the reststrahlen features.

*Figure 2.22* illustrates directional hemispherical reflectance spectra of selected feldspar minerals including Na-plagioclase (albite) and the alkali feldspars, microcline (K), sanidine (K/Na) and orthoclase (K/Na). These spectra were of coarsely crystalline samples (ASTER, 2000). All show a similar reflectance doublet near 8.5 μm, though at slightly different wavelengths. The main differences exist in the 9-10 μm regions. For example, microcline and albite show a small peak at 9.2 μm whereas the other two feldspars show only a trough. Sanidine and orthoclase show a single asymmetric peak near 9.5 μm. In contrast, microcline has twin peak at 9.5 and 9.8 μm whereas albite has twin peaks at 9.6 and 10.0 μm.
c. Garnets

In Figure 2.23, andradite and grossular spectra have the longest wavelength (longer than 9.4 μm) Christiansen Frequencies (reflectance approaches 0 because the refractive indices of the transmitting medium and the material of interest are the same) compared with all the other selected silicate minerals. These garnets also show major, broad reflectance peaks in the 10-12 μm region related to Si-O ν3 vibrations, with a pronounced narrow trough centered near 11.4 μm between them.

Between these two series: The TIR spectra show a pronounced shift in the position of the Christiansen Frequency and the other reststrahlen bands by up to 1.0 μm, though all share the same spectral shape. For example, the Christiansen Frequency shifts from pyrope (8.9 μm) to almandine (9.2 μm) to grossular (9.4 μm) to andradite (9.6 μm) while the minimum between the two Si-O ν3 vibration-related peaks shifts from pyrope (10.6 μm) to almandine (10.8 μm) to grossular (11.2 μm) to andradite (11.6 μm).
d. Pyroxenes

Figure 2.25 presents laboratory bidirectional reflectance spectra of the three clinopyroxenes, diopside (CaMg[SiO$_3$]$_2$), hedenbergite (CaFe[SiO$_3$]$_2$) and augite (Ca[Mg,Fe][SiO$_3$]$_2$[38]). There is complete solid solution between the Ca-rich pyroxenes, diopside (Mg-rich) and hedenbergite (Fe-rich) and even with the less Ca-rich augite/ferroaugite. The TIR spectra (Figure 2.25) show diagnostic clinopyroxene TIR spectral features (emissivity lows) at 8.8, 10.4 and 10.9 μm. However, unlike the garnets, there is little evidence from these library spectra that there exist variations in spectral behavior related to changes in solid solution chemistry.

Table 1: XRD 2-d spacings for the 420 hkl reflection of “pure” garnet minerals.

<table>
<thead>
<tr>
<th>Garnet mineralogy</th>
<th>XRD 2-d spacing (420 hkl peak)</th>
<th>Angstroms?</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pyrope</td>
<td>2.562</td>
<td></td>
</tr>
<tr>
<td>Almandine</td>
<td>2.569</td>
<td></td>
</tr>
<tr>
<td>Spessartine</td>
<td>2.600</td>
<td></td>
</tr>
<tr>
<td>Grossular</td>
<td>2.647</td>
<td></td>
</tr>
<tr>
<td>Manganan andradite</td>
<td>2.620</td>
<td></td>
</tr>
<tr>
<td>Uvarovite</td>
<td>2.684</td>
<td></td>
</tr>
<tr>
<td>Andradite</td>
<td>2.696</td>
<td></td>
</tr>
</tbody>
</table>
In summary, the VNIR, SWIR and TIR regions are most useful for mapping surface mineralogy because these wavelengths are sensitive to a wide range of diagnostic EMR-material interactions. In particular:

1. The mineral-spectral features in the VNIR are largely related to the transfer of electrons between energy levels of constituent elements, especially the transition metal Fe, Mn and Cr;

2. The mineral-spectral features in the SWIR are largely related to the overtones and combination tones of vibrations of octahedrally coordinated cations (typically Al, Fe, Mg) boned with OH groups;

3. The mineral-spectral features in the TIR are largely related to fundamental vibrations (bends and stretches) of Si-O bonds in various structural environments.

### 2.1.3 Mineral information quantitative extraction

#### 2.1.3.1 Major Spectral Features of Minerals

Diagnostic absorption features of hydroxyl mineral groups in the SWIR

- **Al(OH):** 2170 - 2210 nm
  - Topaz, Pyrophyllite, Kaolinite, Montmorillonite, Muscovite, Illite
- **Mg(OH):** 2300 - 2400 nm
  - Chlorite, Talc, Epidote, Amphibole, Antigorite, Biotite, Phlogopite
- **Fe(OH):** 2250 - 2300 nm
  - Jarosite, Nontronite, Saponite, Hectorite
- **Si(OH):** 2240 nm (broad)
  - Opaline silica
The spectral features of minerals (in the wavelength range considered here) are the result of vibrational processes. Their number, intensity and shape are dependent on atomic masses, interatomic force fields and, particularly, molecular geometry. One goal of the spectroscopist is to quantitatively describe the vibrational process so that the origin of each absorption band can be understood. Sophisticated calculations have been made and they are consistent with observation, at least for the simpler minerals (e.g.), although not necessarily correct or final. Even if a vibrational mode were understood precisely, it is virtually impossible to describe such a motion simply and concisely for such complex structures as silicates. Consequently, one must rely on some very general description, such as "Si-O symmetric stretch," to describe all those vibrations which predominantly involve the symmetric expansion and contraction of the silicon-oxygen bonds. Using such simplified visualizations, we can successfully generalize about the spectral behavior of minerals. For example, lighter atoms vibrate at higher frequencies (shorter wavelengths) than heavier atoms when substituted into the same structure. Higher bond strengths also result in higher frequencies of vibration, and this change in bonding in silicates is related to the degree of polymerization of the Si-O4 ion. This results in a systematic change in wavelengths of the fundamental vibration bands of silicates as the framework structure ultimately gives way to isolated tetrahedra. Finally, bond-stretching vibrations in covalent structures lie at higher frequencies than bending modes, and such internal molecular vibrations typically lie at higher frequencies than lattice modes.

The most prominent features in the infrared spectra of minerals can be understood in the context of the generalizations outlined above and are described below for different types of minerals[39]. In particular, we point out those bands seen in reflectance or emittance that are not apparent in the transmittance spectra typically studied by others. This discussion of the origins of spectral features is not repeated in the text for each mineral, because it would prove highly repetitious for the relatively well-understood bands, such as the fundamental internal molecular vibration bands of the minerals and associated water and hydroxyl. Those bands can easily be identified in the spectra of each mineral on the basis of the discussion below. The attribution of more complex features due to overtones and combination tones of the internal vibrations and lattice modes is a more speculative matter, even for the simplest of minerals. Such speculation would also be repetitious and is not the function of this work. Farmer (1974) discusses the spectral features of minerals at length [31], and Farmer and Palmieri (1975) provide an exhaustive list of references categorized by mineral. Estep-Barnes (1977) presented a good review of the major spectral features of minerals, accompanied by an extensive bibliography. The interested reader is referred to these works for the best information on the subject of detailed band assignments.
Silicates:

The most intense spectral features of silicates, occurring between 8 and 12 micrometers, are generally described as due simply to fundamental asymmetric Si-O-Si stretching vibrations, but Si-O-Al stretching vibrations may also contribute when aluminum is part of the crystal lattice (for the classic Si-O-Si stretching feature, see the 9.2 micrometers band in quartz). The appearance of these features typically changes in reflectance because of the role of the refractive index in scattering (see The Role of Surface and Volume Scattering, below). The weak side band near 8.5 micrometers in the transmittance spectrum of quartz, for example, becomes a well-defined lobe of a prominent reflectance doublet between 8 and 10 micrometers. The reflectance spectrum of a quartz glass displays a much weaker short-wavelength lobe, which in some cases of shocked quartz we have seen is reduced to a shoulder. This simplification of glass spectra of minerals is well known and is attributed generally to broadening of the bands [31]. However, broadening would not appear to explain the reduced intensity of the 8.5 micrometers band in the spectrum of glass compared to that of crystalline quartz.

An alternative explanation is that the short-wavelength lobe of the strong quartz reflectance doublet is not due entirely to internal molecular vibrations but depends to some extent on long-range order. Whatever the details of their origin, these most intense features fall in the 8-14 micrometers atmospheric window, making them the most useful for terrestrial remote sensing of silicates.

The second most intense silicate bands are broadly characterized as O-Si-O deformation or bending modes, which occur in the 18-25 micrometers region. Again, aluminum and, indeed, other cations may contribute additional band structure in this region [31]. The relative intensities of the two quartz bands in this spectral region appear unchanged in reflectance compared to transmittance, but have been shifted about 1 micrometer to shorter wavelength by the interaction of absorption coefficient and refractive index on the scattered light, which is typical. The weaker feature occurring at 18.3 micrometers in reflectance completely disappears in the spectrum of fused silica, indicating such a strong dependence on long-range order that it must be due to a lattice vibration.

Weaker bands in quartz spectra between 12 and 15 micrometers have been attributed to symmetric Si-O-Si stretching vibrations. When some of the silicon atoms are replaced by aluminum, as in the feldspars, additional Si-O-Al stretching vibrations are added over a longer wavelength range. For example, albite displays eight highly characteristic bands in its spectrum between 12 and 20 micrometers. Again, such bands are greatly simplified or eliminated in the spectra of glasses.

Additional weak bands are displayed as troughs between 3 and 7 micrometers. Such bands in silicate spectra have been largely ignored because they are usually too
weak to be seen in transmittance spectra. However, they can be very useful in the spectral identification of fine particulate minerals and rocks, where they are quite prominent. Because they have not been assigned with any certainty, we refer to such bands simply as overtone/combination tone bands of internal and lattice modes.

**Carbonates:**

The strongest bands of carbonates are due primarily to fundamental internal molecular vibration bands of the CO3 ion, which are well understood. Carbonates typically display a strong band near 7 micrometers due to asymmetric C-O stretching vibrations and weaker bands near 11.4 and 14.3 micrometers due to bending modes, which can be seen in the spectrum of calcite. Very weak bands in the transmittance spectrum to shorter wavelength than 7 micrometers are strongly displayed as troughs in the reflectance spectrum of particulate calcite. Because of their relative visibility in transmittance spectra, these weak bands have been the subject of study and appear to be due to combination tones of internal and lattice modes.

**Sulfates:**

The sulfate ion displays a group of intense stretching fundamentals near 8.7 micrometers and two or more bending modes near 16 micrometers, as can be seen in spectra of gypsum and anhydrite. Again, the weaker features in transmittance spectra of sulfates at shorter wavelength than the strong stretching fundamental are strongly displayed in reflectance spectra of particulate samples. The complex feature near 4.6 micrometers appears to be a combination tone of the sulphate ion, perhaps accompanied by water combination tones [40]. The features near 2.8 and 6.2 micrometers are due to water, the spectral features of which are discussed separately below.

**Oxides:**

The metal-oxygen stretching vibration bands in oxides occur at longer wavelength than the Si-O features (e.g., chromite). An interesting aspect of these features is that, because of the intense dipole oscillations induced by the vibrations of highly ionic oxides, their powder spectra are profoundly modified by the shape and size of the particles. Thus, it is sometimes uncertain whether variations in powder spectra given by different specimens of a given compound are due to real differences in purity or phase, or merely to shape and size. A case in point is provided by spectra of our two goethite samples.
Sulfides:

Most metal-sulphur vibration bands lie beyond our wavelength range in the far-infrared. We have included two examples (pyrite, and pyrrhotite) that do show bands within our wavelength range.

Water and Hydroxyl:

The most common vibration bands in minerals are due to water and hydroxyl, the spectral features of which have been thoroughly reviewed by Aines and Rossman. When water is not fixed in a crystal lattice but is hydrogen-bonded to other water molecules, it results in a broad spectral feature centered near 2.9 micrometers due to O-H stretching vibrations and another near 6.1 micrometers due to H-O-H bending vibrations. Such water may be present in fluid inclusions, as interlayer water in sheet silicates, or as water of hydration. Water in a crystalline environment produces sharper O-H stretching absorption features than occur in the liquid water spectrum, which typically also occur at a shorter wavelength. Multiple O-H stretching vibrations can result when water is present at several sites in the crystal lattice. Beryl and cordierite, for example, contain water that resides at specific sites in channels parallel to the C axis. These minerals are also interesting because they typically have CO2 trapped in these channels, which produces sharp bands near 4.3 micrometers.

Minerals containing hydroxyl without water display O-H stretching features near 2.7 micrometers but lack the broad feature at 2.9 micrometers and the H-O-H bending mode at longer wavelength. A good example is kaolinite, which has no interlayer water. Most often, however, minerals display a combination of hydroxyl and molecular water bands, as in the case of antigorite.
Many minerals contain a trace of OH and water, although this is not reflected in their chemical formulae. A good example is quartz, which typically displays multiple sharp O-H stretching features superimposed on a weak broad water band. The broad water band is probably due to a small amount of liquid water in fluid inclusions. The sharper hydroxyl features are associated with hydroxylated alkali metals that serve to balance charges when aluminum substitutes for silicon. In addition to the fundamental O-H and H-O-H features commonly seen in the spectra of minerals in the 2-7 micrometers region, a variety of significant metal cation-OH bands can be found at longer wavelength, especially in clay minerals. Kaolinite, for example, displays a prominent Al-OH band near 11 micrometers. OH lattice vibrations are typically seen at still longer wavelengths, such as the 16-micrometers feature in the spectrum of antigorite.

Water and hydroxyl bands are spectrally important because most silicate minerals capable of doing so have undergone incipient alteration to hydrous phases and/or contain fluid inclusions, even when appearing quite fresh, because of the ubiquity of water in the terrestrial environment. This is in marked contrast to other environments, such as that of the moon. It should be pointed out that water and hydroxyl are usually not present in large amounts where they are not part of the mineral stoichiometry. However, spectral features due to water and hydroxyl may be very prominent, especially in reflectance spectra of fine particulate materials. This is due to the enhancement of such absorption bands by the increased scattering associated with fine particle size, which is discussed below. Thus, an estimate of the abundance of water and hydroxyl relative to other phases can best be obtained from transmittance spectra.
2.1.3.2 Mineral spectral absorption mechanism

Figure 2.27 VNIR spectra of iron-oxide bearing minerals vs. other major rock forming minerals

Figure 2.28 Vibrational-Energy-Level diagrams for the water molecule and a corresponding infrared absorption spectrum
The Colors of Minerals

1) Metal ions cause the color of many common and uncommon minerals.

2) Intervalence Charge Transfer, involving metal ions in mixed oxidation states is another important factor in the coloration of minerals. Most commonly, we encounter minerals with the Fe$^{2+}$ - Fe$^{3+}$ interaction and with the Fe$^{2+}$ - Ti$^{4+}$ interaction.

3) Colors from natural ionizing radiation are frequently encountered in nature. Most common minerals have had a long history of exposure to ionizing radiation from natural radiation sources in rocks. A variety of minerals can also be colored by artificial irradiation that enters the commercial market in the form of colored gemstones.

4) Physical effects such as diffraction also cause colors in minerals. The color of gem opal is the result of diffraction as is the color of certain crystals of labradorite feldspar.

5) Semiconducting minerals have band gaps and it often result in intense colors. Numerous sulfides are examples of this.

2.2 Hyperspectral Data Processing

2.2.1 Characteristics of Hyperspectral Data

Recent advances in remote sensing and geographic information has led the way for the development of hyperspectral sensors. Hyperspectral remote sensing, also known as imaging spectroscopy, is a relatively new technology that is currently being investigated by researchers and scientists with regard to the detection and identification of minerals, terrestrial vegetation, and man-made materials and backgrounds[41, 42].

Physicists and chemists have used imaging spectroscopy in the laboratory for over 100 years for identification of materials and their composition. Spectroscopy can be used to detect individual absorption features due to specific chemical bonds in a solid, liquid, or gas. Recently, with advancing technology, imaging spectroscopy has begun to focus on the Earth[43]. The concept of hyperspectral remote sensing began in the mid-80 and to this point has been used most widely by geologists for the mapping of minerals. Actual detection of materials is dependent on the spectral coverage, spectral resolution, and signal-to-noise of the spectrometer, the
abundance of the material and the strength of absorption features for that material in the wavelength region measured[16].

Hyperspectral remote sensing combines imaging and spectroscopy in a single system that often includes large data sets and requires new processing methods. Hyperspectral data sets are generally composed of about 100 to 200 spectral bands of relatively narrow bandwidths (5-10 nm), whereas multispectral data sets are usually composed of about 5 to 10 bands of relatively large bandwidths (70-400 nm).

Hyperspectral imagery is typically collected (and represented) as a data cube with spatial information collected in the X-Y plane, and spectral information represented in the Z-direction.

![AVIRIS hyperspectral data cube over Moffett Field, CA](image)

2.2.2 Processing of Hyperspectral Data

Pre-processing

Pre-processing generally is conducted by the manufacturers, institute/agency or commercial company that maintains and operates the instrument. In most cases the user is provided with at-sensor radiance data and the necessary instrument characteristics (e.g., spectral response functions, band passes etc.) needed for further analysis. The on-ground calibration of an VIS / TIR imaging spectrometer consists of a sequence of procedures providing the calibration data files and ensuring the radiometric, spectrometric and geometric stability of the instrument:

• measurement of noise characteristics of the sensor channels

• measurement of the dark current of the channels

• measurement of the relative spectral response function of the channels
• derivation of the effective spectral bandwidth of the channels

• definition of the spectral separation of the channels

• measurement of the absolute radiometric calibration coefficients (the "transfer functions" between absolute spectral radiance at the entrance of the aperture of the sensor and the measured radiation dependent part of the output signal of each channel)

• definition of the Noise Equivalent Radiance (NER) and the Noise Equivalent Temperature Difference (NE DeltaT) of the channels

• measurement of the Instantaneous Field of View (IFOV), the spectral resolution and the deviations in the band-to-band registration.

**Atmospheric Correction**

Raw calibrated imaging spectrometer data have the general appearance of the solar irradiance curve, with radiance decreasing towards longer wavelengths, and exhibit several absorption bands due to scattering and absorption by gasses in the atmosphere. The major atmospheric water vapor bands (H2O) are centered approximately at 0.94 um, 1.14 um, 1.38 um and 1.88 um, the oxygen (O2) band at 0.76 um, and carbon dioxide (CO2) bands near 2.01 um and 2.08 um. Additionally, other gasses including ozone (O3), carbon monoxide (CO), nitrous oxide (N2O), and methane (CH4), produce noticeable absorption features in the 0.4-2.5 um wavelength region. The effect of atmospheric calibration algorithms is to re-scale the raw radiance data provided by imaging spectrometers to reflectance by correcting for atmospheric influence thus shifting all spectra to nearly the same albedo. The result is a data set in which each pixel can be represented by a reflectance spectrum, which can be directly compared to reflectance spectra of rocks and minerals acquired either in the field or in the laboratory. Reflectance data obtained can be absolute radiant energy or apparent reflectance relative to a certain standard in the scene. Calibration to reflectance can be conducted to result in absolute or relative reflectance data.

Radiation reaching the sensor can be split into four components: path radiance, reflected diffuse radiance, reflected direct radiance, and reflected radiance from neighborhood. Radiative transfer RT codes model the atmosphere's optical behavior given user defined boundary conditions. The inverse problem of atmospheric correction of imaging spectrometer data with the aim of obtaining radiance and/or reflectance at the ground surface can be achieved in three ways:
1. Empirical correction methods to obtain apparent surface reflectance

2. Use of RT codes to obtain absolute reflectance

3. In-flight calibration of airborne optical sensors

It should be noted that empirical approaches such as those listed above only approximate the highly variable processes in time and space in the atmosphere controlling the transfer of radiance to and from the Earth’s surface to the sensor.

Radiometric Correction

Hyperspectral imaging sensors collect radiance data from either airborne or spaceborne platforms which must be converted to apparent surface reflectance before analysis techniques can take place. Atmospheric correction techniques have been developed that use the data themselves to remove spectral atmospheric transmission and scattered path radiance. There are seven gases in the Earth’s atmosphere that produce observable absorption features in the 0.4 - 2.5 micron range. They are:

- Water vapor,
- carbon dioxide,
- ozone,
- nitrous oxide,
- carbon monoxide,
- methane,
- and oxygen.

Approximately half of the 0.4 - 2.5 micron spectrum is affected by gaseous absorption is illustrated below in Figure 2.30. For this reason, the ATREM 3.0 (Atmosphere Removal Program) developed by the Center from the Study of Earth from Space (CSES) at the University of Colorado can be used to remove the effects of the atmosphere from AVIRIS or HYDICE imagery. ATREM is available via anonymous ftp at cses.colorado.edu from the pub/atrem directory.
Figure 2.30 Solar Spectrums with Atmospheric Absorptions

Minimum Noise Fraction (MNF)

MNF (minimum noise fraction) rotation (using principal components calculations) is used to show the variation between bands in an image. This is a statistical method which works out differences in an image based on pixel DNs in various bands. Mathematically, this uses eigenvectors and eigenvalues to work out the principal vectors and directions of the data loud (collection of data values for the image). The idea is to show the differences between what the sensor is picking up in different bands rather than where different bands are recording the same thing i.e. reducing redundancy. The calculations also identify noise in the image. After doing this analysis you can then go and do some band ratios, compare to your MNF or principal components image, and perhaps assign each MNF band to some feature or characteristic.

While hyperspectral imagery is capable of providing a continuous spectrum ranging from 0.4 to 2.5 microns (in the case of AVIRIS) for a given pixel, it also generates a vast amount of data required for processing and analysis. Due to the nature of hyperspectral imagery (i.e. narrow wavebands), much of the data in the 0.4-2.5 micron spectrum is redundant.

A minimum noise fraction (MNF) transformation is used to reduce the dimensionality of the hyperspectral data by segregating the noise in the data. The
MNF transform is a linear transformation that is essentially two cascaded Principal Components Analysis (PCA) transformations. The first transformation decorrelates and rescales the noise in the data. This results in transformed data in which the noise has unit variance and no band-to-band correlations. The second transformation is a standard PCA of the noise-whitened data.

For this particular example, an AVIRIS frame over the Kennedy Space Center was radiometrically corrected using ATREM and a MNF transformation was performed on the ATREM-corrected imagery. In this particular frame, the first 14 eigenvectors of the MNF transformation contain coherent information, which can be used for further processing.

Figure 2.31 Eigenvectors 1, 2, & 3 of MNF Transform Data

Figure 2.32 Eigenvectors 6, 9, & 12 of MNF Transform data

Pixel Purity Index

The Pixel Purity Index (PPI) is a processing technique designed to determine which pixels are the most spectrally unique or pure. Due to the large amount of data, PPI is usually performed on MNF data that has been reduced to coherent images. The most spectrally pure pixels occur when there is mixing of endmembers. The PPI is computed by continually projecting n-dimensional scatterplots onto a random vector. The extreme pixels for each projection are recorded and the total number of hits is stored into an image. These pixels are excellent candidates for selecting endmembers that can be used in subsequent processing.

Principal components

Use principal components to produce uncorrelated output bands, to segregate noise components, and to reduce the dimensionality of data sets. Because multispectral data bands are often highly correlated, the Principal Component (PC) Transformation is used to produce uncorrelated output bands. This is done by finding a new set of
orthogonal axes that have their origin at the data mean and that are rotated so the
data variance is maximized. PC bands are linear combinations of the original spectral
bands and are uncorrelated. You can calculate the same number of output PC bands
as input spectral bands. The first PC band contains the largest percentage of data
variance and the second PC band contains the second largest data variance, and so
on. The last PC bands appear noisy because they contain very little variance, much of
which is due to noise in the original spectral data. Principal Component bands
produce more colorful color composite images than spectral color composite images
because the data is uncorrelated.

Decorrelation Stretch

Decorrelation stretch is another way to enhance images. It is especially useful when
viewing bands that are highly correlated (e.g. combinations of the TIR or SWIR
bands). For example, the TIR bands 10, 12, and 13 are highly correlated and produce
a fairly a dull RGB image. This sort of image is difficult to interpret and not
particularly useful. Applying decorrelation stretch essentially stretched each band
such that the minimum correlation between bands is shown and therefore the
decorrelations, i.e. areas of the spectrum where the bands are not correlated, are
highlighted. It is another way to reduce redundancy in the image.

2.2.3 Processing Systems of Hyperspectral Data at Home

and Abroad

Many software tools are available for the preparation and exploitation of
hyperspectral data. Two common, commercially available analytical software tools
are ENVI™ and ERDAS.

ENVI is a software tool that is used to analyze and display multispectral,
hyperspectral, or radar remote sensing data. ENVI has no limits on file size or
number of bands that can be analyzed during any given processing session. ENVI is
used to process data such as LANDSAT, SPOT, and RADARSAT, while also accepting
data from EarthWatch, ORBIMAGE, and Space Imaging. Figure 5.10 shows a user
interface and sample imagery window from ENVI. ENVI has tools to extract spectra,
reference spectral libraries, and analyze high spectral resolution image datasets from
many different sensors. ENVI is written entirely in Interactive Data Language (IDL),
which is an array-based language that provides integrated image processing and
display capabilities.

ERDAS from Leica Geosystems GIS and Mapping, LLC and the corresponding spectral
analysis tool IMAGINE 44 contain algorithms and other industry recognized
preprocessing techniques for hyperspectral data analysis. ERDAS also processes
information from many sensor systems including AVIRIS and Hyperion. ERDAS creates material mapping information from the spectral data with minimal user interaction.

MATLAB is a computer language used to develop algorithms, interactively analyze data, view data files, and manage projects. MATLAB solves technical computing problems faster than traditional programming languages, such as C, C++, and Fortran, and MATLAB code can be integrated with other languages and applications. MATLAB includes development tools that implement algorithms, including the MATLAB Editor, which provides standard editing and debugging features, such as setting breakpoints and single stepping; M-Lint Code Checker, which analyzes the code and recommends changes to improve its performance and maintainability; MATLAB Profiler, which records the time spent executing each line of code; and Directory Reports, which scan all the files in a directory and report on code efficiency, file differences, file dependencies, and code coverage. The graphics features that are required to visualize hyperspectral data are available in MATLAB. These include 2-D and 3-D plotting functions, 3-D volume visualization functions, and tools for interactively creating plots. You can customize plots by adding multiple axes, changing line colors and markers, adding annotation and legends, and drawing shapes.

A hyperspectral image processing and analysis system (HIPAS) has been developed by Jinnian Wang’s research group in the Institute of Remote Sensing Applications of the Chinese Academy of Sciences. The HEAS, built on Interactive Data Language (IDL) and implemented on Windows NT workstations, meets the requirements for the rapid preprocessing of imaging spectrometer data and easy prototyping of algorithms. Integrated with a spectral library, which was implemented on the FoxPro, a popular database environment in the Windows NT platform, the spectral analysis model was established to support hyperspectral image analyses. Based on the HIPAS, some hyperspectral remote sensing application studies were completed in China. These included mineral identification, agriculture investigation, urban mapping, and the study of wetland vegetation.

2.3 Mineral mapping

2.3.1 Concept of mineral mapping

Planetary surfaces are complex and the Earth’s surface is probably the most complex in our solar system, showing varied geology, oceans, ice caps, abundant life and anthropogenic influences. Other planets have different geology and different surface compositions. In order to understand our own planet as well as others, we produce maps of materials and other measurable quantities. Mineral spectral mapping is a technique based on Hyperspectral Remote Sensing, and now is practicality on the Short Wavelength Infrared. Imaging spectroscopy is a tool that can be used to
identify and spatially map materials based on their specific chemical bonds. Spectroscopic analysis requires significantly more sophistication than has been employed in conventional broad-band remote sensing analysis. In producing materials maps, robustness is vital. If a sensor is flown over the same site with minor changes to the instrument spectral sampling, spectral band pass, and spatial resolution, the materials mapped should still be the same. If the sensor is flown over a geologically different region, and the same minerals exist as in other areas, those minerals should be similarly detected and accurately mapped. When mapping materials in response to environmental or other disasters where lives, health, and economic impacts play major roles, mapping accuracy becomes more important.

2.3.2 Processing of Mineral Exploration and Geological Assessment

Processing of hyperspectral data is carried out to produce various image products through a sequence as described below:

LEVEL 1: Preprocessing

- Level 1A: Conversion of Raw DN images to radiance imagery and derivation of geometric correction files
- Level 1B: Conversion of radiance to reflectance data.
- Level 1C: Production of geometrically, cross track and radiometrically corrected mosaic from which further products are derived

LEVEL 2: Photo Interpretation Products (images that do not map mineral uniquely)

- Overview Color composites: Landsat TM 432 equivalent, true and false color images
- MNF Color Composite Images: 2-4 color composites are produced
- Mineral Class Images that map distribution of: MgOH/CO$_3$, FeOH, SiOH, AlOH, Argillic, Sulfate, Iron Oxides minerals but not specific minerals, produced using decorrelation stretching

LEVEL 3: Mineral Abundance and Mineral Chemistry Image Maps

- SWIR and VNIR Mineral Abundance Mapping:
- Mineral abundance images are produced from end-member un-mixed images, Match Filtered and Logical Operator processes and are presented as: Thresholded Greyscale, Thresholded Pseudo Coloured, Mineral Map RGB Colour Composite and Rule Classified Multi Mineral Maps Mineral abundance images are produced from end-member un-mixed images.
- Pseudo Colored Absorption Minima Wavelength Shift Mapping is carried
out by using a polynomial curve fitting routine to determine the wavelength position of an absorption feature of interest in each pixel and creating an image of these values. This technique can be used to determine mineral composition such as the Illite Al content, FeOx type and Carbonate and Chlorite composition.

LEVEL 4: Detailed Integrated Analysis

After the customer has examined the delivery products, which are produced as information images in formats for input into GIS (ECW, GeoTiff, JPEG and if vectors shape files), further refinement of the processing can be carried out interactively with the customer.

Some Mineral Targeting examples of models are:

i) Mapping zoning in porphyry systems
ii) Mapping Argillic and Advanced Argillic minerals to target epithermal deposits
iii) Mapping changes in carbonate composition in Calcrete U and MVT deposit
iv) Mapping change in white mica – illite Al content associated with Archean gold deposits and unconformity U also location of Chlorite and Dravite.
v) Locating Mg-OH minerals – Talc, Serpentine and Saponite that highlight kimberlite etc
vi) Gibbsite mapping for Bauxite deposits Gibbsite mapping for Bauxite deposits

OUTPUT IMAGES that are result of Level 2 and 3 (underlined) processing are written to ENVI, ER Mapper, ECW, JPEG and GeoTiff formats. The mineral mapping and mineral chemistry images can be presented as overlays onto a grayscale background and individual areas of mineral occurrence can be output as shape files.

2.3.3 Applications of mineral mapping

The minerals mapping application provides an in-depth view of minerals activities on state trust lands. This includes lease information, well locations, and geological information, as well as other pertinent information. Maps of the Earth’s surface can depict many themes, including those in geology, ecosystems, environmental hazards, land management and global change. Geologic mapping can include the depiction of geologic formations (thus providing information on ages and placements of units through geologic time), soils, mineral occurrences, faults, mineralized zones and aggregate for building materials. Environmental applications can include acid-rock drainage, oil or toxic waste spills, water quality and other distributions[44]. Geologic hazards maps can include volcanic eruption potential, swelling clays, fault zones and
landslide hazards. The need for accurate and more detailed maps has never been greater, which drives the requirement for more advanced information such as that from imaging spectrometers.

Maps derived from imaging spectroscopy data have already proven their value. Examples include:

Oxidation of sulfides in the Leadville mining district in the central Colorado Rockies releases lead, arsenic, cadmium, silver and zinc into snow melt and thunderstorm runoff, which drains into the Arkansas River. The Arkansas River is a main source of water for Front Range urban centers and agricultural communities. Maps of pyrite and jarosite, derived from imaging spectroscopy data, showed the source regions of acidic water. The maps helped to accelerate the cleanup efforts by 2.5 years and saved $2 million in remediation costs.

Cuprite, Nevada is one of the premiere sites in the world for field-testing the accuracy of new sensors and spectral mapping techniques [14, 45-49]. This site is ideally suited for remote sensing because of its diverse alteration mineralogy, excellent rock exposures, sparse vegetation, dry climate and easy access. The hydrothermal alteration at Cuprite consists of two barren advanced-argillic lithocaps, straddling U.S. Highway 95. These systems were active between 6.2-7.6 Ma, most likely a result of volcanic activity related to nearby Stonewall caldera, now a resurgent volcanic dome 5 km east of Cuprite. Mineral maps made from AVIRIS data show a wide variety of alteration and rock-forming minerals including Na-K alunites, buddingtonite, calcite, chalcedony, chlorite, dickite, goethite, halloysite, hematite, jarosite, kaolinite, montmorillonite, muscovite (Al-Mg-Fe compositional series), nontronite, opal and pyroxene. The first natural occurrence of the NH4-mineral buddingtonite was discovered with imaging spectroscopy at Cuprite. Tetracorder mineral maps reveal that the western relict alteration center lacks a siliceous cap, has a propylitic remnant surrounded by an advanceargillic alunite zone, and that the system was deeply eroded, exposing the high temperature kaolinite polymorph dickite and a pyrite-rich zone. Mineral maps indicate that the eastern relict alteration center has an extensive siliceous cap surrounded by an advance-argillic alunite zone, lacks a propylitic remnant (at least at the present level of exposure), has extensive kaolinite zones lacking dickite and has volumetrically insignificant jarosite, all consistent with present exposure near the top of the hydrothermal system. Apparently, the hydrothermal systems at Cuprite formed at different times with activity first in the western center and then spreading to the eastern center.

Rapid-response materials maps of the World Trade Center disaster were produced from imaging spectroscopy data that showed the location and temperatures of fires and also showed that there was no widespread distribution of asbestiform minerals or other toxic materials in the dust/debris from the collapse of buildings, in agreement with ground-sample analyses. However, the dust was found to generate
high pH, so maps of the dust indicate that hazard, which caused eye irritation and respiratory problems. The maps also showed asymmetric debris distribution indicating a non-symmetric collapse of the buildings.

Iron ore is the third-largest export earners in Australia and Port Hedland, located on the North West coast in the Pilbara region of Western Australia, which is one of the largest port handling facilities. The processing, blending, and handling of ores produces a considerable amount of dust. Given the proximity of the Port Hedland township to surrounding mangroves ecosystem, managing dust is a top priority for BHP Billiton Iron Ore (BHPBIO, the main user of the facility) and is a significant concern of the community and regulators. BHPBIO is required under its ministerial conditions for the operation of the facility to monitor the effects of dust on the surrounding ecosystem, and BHPBIO has invested heavily in monitoring and controlling dust emissions. This includes the implementation of a series of monitoring and suppression programs over the years, including the use of non-directional gauges to collect dust data from the mangroves in 1996. These gauges are currently accepted as the standard tool for monitoring ambient dust fallout even though they were developed in the 1920s. Ten sites, each with four gauges, were established, but the many risks and physical difficulties of working in the mangroves, such as deep mud and tides, the threat of Ross-River virus from disease infested insects, the labor-intensive nature of regular checking, and especially, the questionable accuracy of the gauges prompted the search for a better method of monitoring and assessing the dust impacts on the mangroves.

Research has been ongoing since 1998 to develop an operational method to generate accurate measurements of dust quantities on mangroves from airborne hyperspectral data. This research included field, laboratory and airborne components. The field and laboratory studies incorporated intensive field studies where independent measurements of dust quantities on the surface areas of leaves were collected concurrent with the reflectance of the leaves. A total of 212 samples were collected to be used in these experiments designed to develop a robust algorithm to generate measurements of quantities of iron oxide dust per area from surface reflectance. The analysis was performed using partial least squares analysis and the algorithm was developed using spectral parameterization of iron oxide diagnostic spectral features. The algorithm was validated using two independent sets of mangrove leaves data collected in the field. The airborne component focused on the reduction of the airborne data to accurate surface reflectance and cross calibration issues between these airborne data and the field and laboratory reflectance to ensure that the results of the laboratory and field studies are transferable to the airborne data. A total of six airborne data sets had been collected over the Port Hedland Harbour from 1998 to 2005. Dust on mangrove maps have been generated for all these data sets and the maps have been validated with independent field measurements. This monitoring system has been recognized by the industry and regulators and is in the process of being incorporated into routine
environmental management system of BHPBIO's port facility.

Hyperspectral Mineral Mapping is a new concept, and it is used to characterize one or some hydrothermal minerals and their relative content on the ground. Satellite-based hyperspectral mineral mapping of the Earth is now possible using NASA's EO-1 Hyperion sensor, launched in November 2000. Hyperion covers the 0.4 to 2.5 micrometer spectral range with 242 spectral bands at approximately 10nm spectral resolution and 30m spatial resolution from a 705km orbit. Comparisons of Hyperion data to airborne hyperspectral data (AVIRIS) show that Hyperion provides the ability to remotely map basic surface mineralogy. Minerals mapped using Hyperion includes calcite, dolomite, kaolinite, alunite, buddingtonite, muscovite (several varieties), hydrothermal silica, and zeolites. Case histories demonstrate the viability of Hyperion as a means of extending hyperspectral mineral mapping to areas not accessible to aircraft sensors.

Imaging spectroscopy plays a key role in planetary exploration. The Mars Global Surveyor (MGS) is currently orbiting Mars with the Thermal Emission Spectrometer (TES), which located deposits of hematite that led to the selection of a Martian landing site with unique geology. The Cassini Visual and Infrared Mapping Spectrometer, VIMS, are currently mapping minerals in the Saturn system, and the Mars Express OMEGA is currently mapping Mars. The Mars Reconnaissance Orbiter is carrying a next-generation spectrometer, CRISM, to Mars to begin mapping in 2006 and NASA's Moon Mineralogy Mapper (M3) will begin assessing lunar resources in early 2008 on board the Indian satellite Chandrayaan-1. The planetary future of imaging spectroscopy is bright, with entire planets being mapped. Similar coverage of the Earth with imaging spectrometers is needed.

High resolution spectral sensing, or hyperspectral surveying, is an advanced remote sensing technique that maps the distribution of surface materials through their spectral signatures. This technology can be applied to material exploration, geological mapping and environmental minesite monitoring. The successful application of this technique depends on determining the surface spectral signature of materials of interest. With this knowledge, image data collected with airborne scanners can be processed to map the distribution of the materials of interest. In geoscience applications this is termed mineral mapping.

Examples of hyperspectral mineral mapping are presented in the following images.
Figure 2.33. False Color Composite Image Mosaic of 5×20km E-W Flight Lines

Figure 2.34. Mineral endmember distribution of Red = Kaolinite/Pyrophyllite, Green = Dickite, Blue = White Mica (Phengite). This image depicts a zone of advanced argillic alteration (red) striking west to east across the center of the area that broadens in the east of the area (red and green). The eastern alteration area is cut by a NS trending ridge of younger/silicified rocks.

Figure 2.35. Mineral Map showing distribution of Red = White Mica (Phengite), Blue = Opaline Silica

Combined use of the VNIR, SWIR and TIR atmospheric windows should therefore allow identification of a wide range of minerals necessary for most geological applications. For example:
1. The VNIR wavelength region is potentially useful for mapping gossans, rich in iron oxides and associated with weathered sulphide occurrences, as well as regolith characterization;

2. The SWIR wavelength region is potentially useful for mapping alteration haloes that comprise minerals like chlorites and white micas in epithermal/porphyry styles of Cu-Au mineralization [27] as well as regolith characterization;

3. The TIR wavelength region is potentially useful for mapping a range of exploration targets. For example, in more weathered environments, mapping silicification associated with epithermal/porphyry alteration [50] may be useful. Similarly, Mn-rich garnets associated with Broken Hill style Pb-Zn-Ag mineralization[51] or Fe-rich garnets in Cu-Zn skarn system [51] can be targeted. In less weathered terrains, pyroxene composition can potentially be used as an indicator for skarn deposits [52] whereas feldspars could be important in mapping granite host rocks or granite-associated mineralizing fluids [53]. For example, the Proterozoic Cu-Au-U mineralization at Olympic Dam [54], rare earth mineralization[55] and Archaean lode Au deposits [56] are all associated with specific types of granites.

Hyperspectral surveys can be used in diamond exploration to locate kimberlitic that are exposed or weathered in areas of residual soil. Surveys need to be conducted during the dry season.
The spectral signature of these minerals, apart from hematite and silica, are characterized by strong absorption minima at ~2300nm and ~2390nm (Figure 2.37). Though not unique to kimberlite detection, anomalous occurrences of these minerals can lead to the discovery of kimberlite, particularly when combined with other exploration data in GIS analysis.

(2) URANIUM EXPLORATION

For uranium exploration, the hyperspectral technology could produce images and mineral maps that improve regional and local geological maps in target areas and locate minerals that are associated with U deposits to:

- Define alteration zones that target unconformity U deposits to assist with ranking radiometric anomalies and locate mineralization that does not outcrop.
- Detect Reibekite that is an indicator of metasomatic deposits.
- Map carbonates dykes and pods that define carbonatites and detect the presence of earth minerals and apatite in these rocks.
- Map regolith associated with paleodrainage calcrete deposits including differentiating calcite from dolomite and potentially locating buried dolomite calcrete from presence of Mg-Smectite.
- Detecting the quartz stockworks (+/- xenotime-rare earth phosphate) and associated alteration clay signatures that define hydrothermal deposits containing rare earths and uranium.
- Mapping graphitic horizons that are associated with unconformity deposits.

Figure 2.38: Calcrete hosted paleodrainage uranium deposit: the boundaries of known mineralized calcrete are shown as white polygons. The predominant mineral that defines these calcretes is calcite (red). Residual illite partially covers some of the calcrete and in the eastern most polygons the presence of dolomite may show a change in calcrete facies.

Narrow-band sensors such as the HyMap imaging spectrometer are capable of detecting spectral absorption in the visible to short-wave infrared specific to some individual minerals. If these minerals are indicative of the type of alteration and present in sufficient quantities at the surface from which solar radiation can be reflected to the sensor, then imaging spectrometers offer the prospect of a valuable, additional source of data for exploration geologist.
Table 2: alteration spectral signature and deposit type

<table>
<thead>
<tr>
<th>Commodity</th>
<th>Deposit Type / Alteration Style</th>
<th>VNIR Minerals</th>
<th>SWIR Minerals</th>
<th>Spatial</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au</td>
<td>Archaean Gold/ Hydric Cells</td>
<td>Goethite, Hydrated FeOx</td>
<td>White mica (Al rich to Al poor &amp; hydration state), pyrophyllite, Fe &amp; Mg chlorite, amphibole</td>
<td>Intersecting cells defined by changes in mica chemistry (gradients) and fracture control.</td>
</tr>
<tr>
<td>Au</td>
<td>High Sulfidation/ Epithermal? Advanced argillic</td>
<td>Goethite, Hydrated FeOx</td>
<td>Alunite, pyrophyllite, kaolinite, dickite, diaspore, opaline silica</td>
<td>Concentric and fracture controlled zonation of alteration minerals.</td>
</tr>
<tr>
<td>U</td>
<td>Unconformity/ Argillic-Propylitic</td>
<td>Hematite</td>
<td>Chlorite, white mica, pyrophyllite, dickite</td>
<td>Zone along unconformity.</td>
</tr>
<tr>
<td>Base Metals</td>
<td>VMS/ Argillic</td>
<td>Goethite, Hydrated FeOx, Jarosite, rozenite</td>
<td>Jarosite, white mica (Al rich to Al poor &amp; hydration state), chlorite, opaline silica</td>
<td>Strike controlled trains of deposits, can be en echelon.</td>
</tr>
<tr>
<td>Base Metals</td>
<td>Porphyry Copper / Propylitic</td>
<td>Hematite</td>
<td>Amphibole, carbonate (Ca-Mg), montmorillonite, nontronite, epidote, Mg &amp; Fe chlorite</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Phyllic (Sericite)</td>
<td></td>
<td>White mica (Al rich to Al poor &amp; hydration state), illite-smectite, kaolinite, quartz.</td>
<td></td>
</tr>
<tr>
<td>Potassic</td>
<td></td>
<td></td>
<td>Biotite, phlogopite, chlorite, vermiculites, anhydrite, gypsum</td>
<td></td>
</tr>
<tr>
<td>Argillic-Advanced Argillic</td>
<td></td>
<td>Hematite</td>
<td>Kaolinite, halloysite, montmorillonite, white mica, dickite, pyrophyllite, alunite, diaspore, topaz</td>
<td></td>
</tr>
<tr>
<td>Supergene Leach Cap</td>
<td></td>
<td>Hematite, goethite</td>
<td>Alunite, jarosite, kaolinite, gypsum</td>
<td></td>
</tr>
</tbody>
</table>

The relative spectral characteristics are as follows:

Figure 2.39: The SWIR spectra shown are a selection of the main alteration minerals as recorded HyMap scanners. Top left: White mica (illites) spectra in which the main absorption at ~2.2um shifts in wavelength with variations in mineral chemistry from Al rich at 2.19um (paragonite) to Al poor at >2.215um (phengite). Top right: Phyllic-Argillic mineral dominated by absorptions at and below 2.2um. Bottom: Propylitic minerals dominated by absorptions beyond 2.25um.
Examples of mineral map are shown as below:

Figure 2.40. INDEX COLOUR COMPOSITE (Hematite, Goethite, Pyrophyllite)

Figure 2.41. OVERVIEW COLOUR COMPOSITE (BANDS 108, 28, 3RGB)

Figure 2.42. MNF COLOUR COMPOSITE (BANDS 5, 4, 2 RGB)
Chapter 3 Hyperspectral data surface mineral mapping

3.1 Spectral Analysis Methods

3.1.1 Field spectral data are spectral features analysis method

1) Spectral derivatives

A spectrum that is the result of applying a derivative transform the data of the original spectrum. Derivatives of spectra are very useful for two reasons[57]:

1). First, derivatives may swing with greater amplitude than the primary spectra. For example, a spectrum suddenly changes from a positive slope to a negative slope, such as at the peak of a narrow feature (see the figure below). More distinguishable derivatives are especially useful for separating out peaks of overlapping bands.

2). Second, in some cases derivative spectra can be a good noise filter since changes in base line have negligible effect on derivatives. For instance, scattering increases with wavelength for some biologically active macromolecules causing an increasing slope of the absorbance baseline.

A common used approximation for the first derivative is: \( \frac{d\alpha}{d\lambda} = \frac{\alpha(\lambda + \Delta \lambda) - \alpha(\lambda - \Delta \lambda)}{2\Delta \lambda} \).

A more accurate approximation of the first and higher order derivatives is presented in thorough explanations by Whitaker1 and Morrey2. Still other methods involve a best fit match to the curve on the features of interest and performing higher order derivatives with numerical analysis.

Derivative spectra yield is good signal-to-noise ratios only if the difference of noise levels at the endpoints of the interval is small enough to yield a noise equivalent \( \Delta \frac{d\alpha}{d\lambda} \) calculation much smaller than the absorbance.
2) Spectral Integral

The canonical spectral integral \([L, \text{eq. } (8)]\) is given by

\[
U_+ (r, r'; t) = \frac{1}{2\pi^2} \int d\xi \frac{A(r, r'; \xi)}{t - \tau(r, r'; \xi)}, \text{Im}\tau < 0 \quad (1)
\]

Where \(r\) and \(r'\) are observation and source point coordinates, respectively, \(C\) is an integration contour along the real axis in the complex spectral \((\xi)\) plane, while \(A\) is the amplitude and \(T\) is the phase of the plane wave spectra that synthesize the analytic signal \(U_r\). The transient field is recovered from \(U_+\) by the relation

\[
U(r, r'; t) = \text{Re} \ U_+ (r, r'; t). \quad (2)
\]

The integral in (1) may be evaluated by two approaches: 1) analytic function theory in the complex \(\xi\) plane, and 2) the real-spectra distributional limit \([L, \text{ eq. } (1\ lb)]\).

Though we emphasize here the evaluation and interpretation of the complex spectral contributions, we shall start with the second approach as employed by Chapman. Encountered below are the spectral quantities; \(\xi_C, \xi_P\) and \(\xi_P\), which identify, respectively, real, upper half-plane complex, and lower half-plane complex time dependent roots of \(t - \tau [\xi(t)] = 0\); branch points at the edges of the visible spectrum; other possible branch points, and pole singularities associated with the spectral amplitude \(A\).
3) Envelope analysis

In recent years there has been an increasing interest in applying cyclostationary analysis to the diagnostics of machine vibration signals. This is because some machine signals, while being almost periodic, are not exactly phase-locked to shaft speeds, and thus even after compensation for speed fluctuation cannot be extracted by synchronous averaging. Typical examples are the combustion events in IC engines, which vary from cycle to cycle, and impulsive signals from faults in rolling element bearings, which are affected by minor but randomly varying slip. Two main tools for the analysis of cyclostationary signals are the two-dimensional autocorrelation function vs central time on the one axis and time displacement around the central time on the other, and its two-dimensional Fourier transform known as the spectral correlation. The latter can be quite complex to interpret, so some authors have suggested integrating it over all frequencies to obtain a Fourier series spectrum vs cyclic frequency. In this paper, it is shown that this gives the same result as a Fourier transform of the average squared envelope of the signal, which is much easier to obtain directly. Not only that, envelope analysis has long been used in the diagnostics of rolling element bearing signals, and some of the experience gained can be carried over to spectral correlation analysis. There is a possibility that the full spectral correlation may still give some advantage in distinguishing between modulation effects due to gear rotations and bearing inner race rotations (even at the same speed) by virtue of the different amounts of randomness associated with each.

For many years, one of the most successful techniques for diagnosing faults in rolling element bearings has been the so-called &envelope analysis', where the envelope of the signal (obtained by amplitude demodulation), rather than the raw signal itself, is frequency analysed to detect the bearing fault frequencies. The reasons for the advantage of this approach have been explained qualitatively, but not quantitatively. One of the aims of this paper is to give a quantitative evaluation of the degree to which information about bearing faults can be extracted by frequency analysing the raw signal. Another is to demonstrate the relationship between the classical envelope analysis (and in particular, analysis of the squared envelope) and spectral correlation analysis, one of the tools used to characterise cyclostationary signals. A third aim is to point out how experience already gained in using envelope analysis can be used to improve results obtained by spectral correlation of cyclostationary signals more generally.

4) Spectral absorption feature parameters

Reflectance spectra of carbonate minerals in the shortwave infrared (SWIR) and thermal infrared (TIR) wavelength regions contain a number of diagnostic absorption features. The shape of these features depends on various physical and chemical parameters. To accurately identify carbonate minerals or rocks in pure and mixed
Carbonate rocks, which are recognized as an important natural resource for construction materials and the cement industry, are sedimentary rocks that mostly consist of calcite (CaCO$_3$) and dolomite (CaMg(CO$_3$)$_2$). These carbonate minerals in the form of limestone also have an economic interest in terms of petroleum geology, because their porosity is a potential storage reservoir for oil and natural gas. The development of porosity in limestone is affected by the sequence of diagenetic processes, which include dolomitization. The dolomitization process involves the placement of calcite by dolomite in the rock when magnesium-rich water permeates through limestone. The process may result in an increase in the porosity of the rock by up to 12%, making it suitable as a natural reservoir for oil. The implications of dolomitization for oil exploration and the importance of dolomite in making cement make it a favorable mineral to be investigated. Besides the interest in oil and gas reservoir characterization, there is an interest in looking into calcite-dolomite mineralogy from an ‘ore geology’ perspective, as carbonates are important pathfinder and alteration minerals associated with calcic skarn deposits, low sulphidation epithermal deposits and porphyry Cu deposits. In addition, coral reefs are under worldwide decline as a result of climate change. Corals are among the species that contribute to carbon sequestration, the capture of carbon dioxide (CO$_2$) from the atmosphere, and act as natural carbon sinks. As they are largely built of carbonate material, more information on its spectral characteristics will help in better species differentiation and in mapping using remote sensing. Carbonate minerals have diagnostic absorption features in the shortwave infrared (SWIR) and thermal infrared (TIR) regions due to vibrational processes of the carbonate ions (CO$_3^{2-}$). In general, carbonate minerals can be distinguished by the presence of two prominent spectral absorption features in the wavelength ranges around 2.50–2.5 Carbonate rocks, which are recognized as an important natural resource for construction materials and the cement industry, are sedimentary rocks that mostly consist of calcite (CaCO$_3$) and dolomite (CaMg(CO$_3$)$_2$). These carbonate minerals in the form of limestone also have an economic interest in terms of petroleum geology, because their porosity is a potential storage reservoir for oil and natural gas. The development of porosity in limestone is affected by the sequence of diagenetic processes, which include dolomitization. The dolomitization process involves the placement of calcite by dolomite in the rock when magnesium-rich water permeates through limestone. The process may result in an increase in the porosity of the rock by up to 12%, making it suitable as a natural reservoir for oil. The implications of dolomitization for oil exploration and the importance of dolomite in making cement make it a favorable mineral to be investigated. Besides the interest in oil and gas reservoir characterization, there is an interest in looking into calcite-dolomite mineralogy from an ‘ore geology’ perspective, as carbonates are important pathfinder and alteration minerals associated with calcic skarn deposits, low sulphidation epithermal deposits and porphyry Cu deposits. In addition, coral reefs are under worldwide decline as a
result of climate change. Corals are among the species that contribute to carbon sequestration, the capture of carbon dioxide (CO$_2$) from the atmosphere, and act as natural carbon sinks. As they are largely built of carbonate material, more information on its spectral characteristics will help in better species differentiation and in mapping using remote sensing. Carbonate minerals have diagnostic absorption features in the shortwave infrared (SWIR) and thermal infrared (TIR) regions due to vibrational processes of the carbonate ions (CO$_3^{2-}$). In general, carbonate minerals can be distinguished by the presence of two prominent spectral absorption features in the wavelength ranges around 2.50–2.55 μm and 2.30–2.35 μm in the SWIR and around 13.70–14.04 μm and 11.19–11.40 μm in the TIR. These features can be used to identify pure and mixed calcite and dolomite in synthetic samples or carbonate rocks, because the absorption band position of calcite is located at a slightly longer wavelength than that of dolomite. Although the absorption band positions of these particular minerals have been observed by multiple researchers, the precise position of calcite and dolomite absorption bands in the SWIR and TIR spectra has been recorded at different wavelengths. There are several factors controlling the position of carbonate absorption bands at the atomic level: cation mass, cation radius, cation and anion valences, cation coordinate number, the gap between cation and anion, and site symmetry. Spectral absorption features of carbonate minerals in the infrared region are also influenced by physical and chemical parameters such as grain size, texture, packing or porosity, carbonate mineral content, and chemical composition (metalion impurity). Previous studies of the effect of particle size on carbonate absorption features in the SWIR revealed that differences in grain size change reflectance values and absorption feature depth, but absorption band position, width, and asymmetry of the features are invariant to grain size. Position, depth, and asymmetry of carbonate absorption feature in the SWIR are displaced by changing the relative amounts of calcite and dolomite composing a sample. The presence of iron in the form of Fe$^{2+}$ in carbonate minerals reduces the reflectance value and depth of the carbonate absorption feature in the SWIR. Although the spectral absorption features of carbonate minerals in the SWIR wavelength region have been extensively studied, they have not been fully explored and observed in the TIR region, particularly with regard to the influences of grain size and carbonate mineral mixtures. We analyze the spectral absorption feature characteristics of calcite and dolomite in both the SWIR and TIR wavelength regions as a function of grain size and calcite-dolomite mixtures. To accurately identify carbonate minerals in pure and mixed forms, it is necessary to analyze the effects of those parameters that change spectral characteristics.

Absorption feature characteristics analysis consisted of determining absorption band position, depth, full width at half maximum (FWHM), and asymmetry, calculated from continuum-removed spectral. The position of the absorption band is defined as the wavelength at which the maximum absorption or minimum reflectance of an absorption feature occurred. The depth of the absorption feature indicates the reflectance value at the shoulders minus the reflectance value at the position of the
absorption wavelength. The FWHM is defined as the width of the spectral feature at half the maximum depth. The asymmetry of the absorption feature represents the logarithm of the ratio of the area right of the absorption position (Area B) to the area left of the absorption position (Area A), where the result of the calculation is zero if the absorption feature towards shorter wavelengths, and a positive value for a skewed absorption feature towards longer wavelength.

![Figure 3.2. Definitions of absorption feature characteristics.](image)

**ABSORPTION FEATURE-BASED CHARACTERIZATION AND MAPPING**

Many researchers have concentrated on the use of specific absorption features in reflectance spectra to identify specific materials [42, 58-61], and have attempted to apply these techniques to imaging spectrometer data [62, 63]. The approach described here, an expert system, has been moderately successful in identifying mineralogy in arid terrains using AVIRIS data. An expert system approach developed at CSES allows automated identification of Earth surface materials based on their spectral characteristics in imaging spectrometer data [45]. This expert system requires that the imaging spectrometer data be calibrated to reflectance because rules for identification are built using laboratory reflectance spectra. Once the data are properly calibrated, the procedure is to treat each pixel individually and sequentially to remove continuum (normalize), binary encode the spectrum [64], extract the features, and compare the binary encoding and features to the binary encoded reference spectrum and the feature rules built from the spectral library of reference materials. The result of these analyses is a new data cube consisting of a single image for each end member contained in the spectral library [45]. These images contain a value for each pixel indicating an empirical probability that a particular material will occur at that location. Probabilities range from 0.0 to 1.0 with
indicating a perfect match. More specifically, the procedure is as follows. A spectral library of laboratory reference spectral reflectance measurements is used to develop a generalized knowledge base for analysis of visible and infrared reflectance spectra. Several libraries are available in the public domain [29]. Spectral features are digitally extracted from a spectral library and numerical analysis and characterization of the digital reflectance measurements are used to establish quantitative criteria for identifying materials. Absorption feature information is extracted from laboratory spectra (and later each image spectrum) using the following automated techniques [45, 63].

1) A continuum is defined for each spectrum by finding the high points (local maxima) and fitting straight line segments between these points.

2) The continuum is divided into the original spectrum to normalize the absorption bands to a common reference. (See Clark and Roush, 1984 for a discussion of division versus subtraction of the continuum).

3) The minima of the continuum-removed spectrum are determined and the 10 strongest absorption features extracted.

4) The wavelength position, depth, full width at half the maximum depth (FWHM), and asymmetry for each of these 10 features are determined and tabulated. The asymmetry is defined as the sum of the reflectance values for feature channels to the right of the minimum divided by the sum of the reflectance values for feature channels to the left of the minimum. The base ten logarithm is taken of this value to maintain linearity. Symmetrical bands thus have an asymmetry value of zero (the area to the left and right of the band center are equal). Bands that are asymmetrical towards shorter wavelength have negative asymmetry, while bands that are asymmetrical towards longer wavelengths have positive asymmetry. The magnitude of the asymmetry value indicates the degree of asymmetry. The information derived from the analysis of the spectral library are interactively reviewed simultaneously in both tabular and graphical format to determine if features extracted from the digital spectra are representative of the material measured or were due to impurities. The four parameters derived using the feature extraction procedure are used in conjunction with published spectral information to determine the critical absorption bands and absorption band characteristics for identification of specific materials. Facts and rules are formulated based on the analysis of the reference spectra. The final step is to apply the rules to an imaging spectrometer data set to automatically identify materials and to map their spatial distributions. The absorption feature positions and shapes of each reflectance spectrum for each picture element (pixel) are characterized using the automated techniques described previously for individual laboratory spectra. The final products of the expert system analysis are a "continuum-removed" cube with "n" bands containing all of the continuum-removed spectra calculated from the reflectance data, a "feature" cube containing the
wavelength positions, depths, FWHMs, and asymmetries for each pixel for the ten strongest absorption features, and an "analysis cube" showing the location and probability of occurrence of the reference materials based on a weighted combination of binary encoding, and feature analysis in the expert system. The analysis cube also contains four images that help with evaluation of the expert system mapping success.

These are 1) the "final decision best end member" image showing the single best match for each pixel, 2) the "sum of decisions" image showing the sum of all probabilities for each pixel, 3) the "number of decisions greater than or equal to 50%" image showing those areas with end members with high probabilities, and 4) the "no match" image showing those areas with maximum probabilities less than or equal to 10%. Interactive display and analyses of the probability images and the additional images described above permits determination of the spatial extent of specific minerals and identification of problem areas where the expert system may have identified multiple minerals, or no minerals at all. These images from the starting point for detailed analyses using techniques such as linear spectral unmixing.

5) Spectral curve simulation

Curve fitting methods are now widely applied both qualitatively and quantitatively to separate overlapped peaks in composite profiles. Nevertheless, the achievement of a good representative fit requires the knowledge of the number of component bands, their positions, shapes and widths. The most important values for input to curve fitting route are the number of bands and their positions. Up to present, there are many methods employed for doing this. Madams and coworkers applied the second or fourth derivative in determining the number and the position of overlapped peaks. However, this kind of determination requires a very good signal-to-noise ratio (SNR) in the original spectra. Fourier self-deconvolution (FSD) is an alternative method for an estimation of parameters in curve fitting. It is shown that the condition of curve fitting is significantly improved as well as the selection of the parameters in FSD becomes even more objective. Unfortunately, there solving ability of FSD is counterbalanced by a number of failings, such as the method still requires good SNR as well as a mathematical model with an appropriate half-width to describe band shape. Apart from these methods, natural computation also was applied to peak detection, yet it is very complicated and time consuming because it needs to learn form lot of samples to establish a model. Wavelet transform is a novel signal processing technique developed from the Fourier transform and has been widely used to signal processing. The main characteristic of wavelet transform is that its time–frequency localization or scale is not the same in the entire time–frequency domain. Thus, wavelets possess multiscale character and are able to adjust their scale to the nature of the signal features. Furthermore, wavelets can be orthonormal and are able to capture deterministic features. Therefore, it can decompose a signal into localized contributions labeled by dilation and translation parameters, and each of the contributions represents the information of different frequency contained in
analyzing signals. Based on this multiscale character, the method of curve fitting using wavelet transform was proposed in this work. Here, wavelet transform was used prior to curve fitting in order to estimate parameters of components in composite profiles, for instance, peak number, half-width and their positions. Again, it also was applied to improve noise level in the original signal in order to make it fit to subsequent fitting. Accordingly, the fitted conditions can be improved to the point that very accurate results could be acquired even for the simulated overlapped bands with higher noise level.

3.1.2 Spectral Matching

Matching spectra is necessary for database searches, assessing the source of an unknown sample, structure elucidation, and classification of spectra. A direct method of matching is to compare, point by point, two digitized spectra, the outcome being a parameter which quantifies the degree of similarity or dissimilarity between the spectra.

1) Spectral Angle Mapper (SAM):

The Spectral Angle Mapper (SAM) is a physically-based spectral classification that uses an n-dimensional angle to match pixels to reference spectra. The algorithm determines the spectral similarity between two spectra by calculating the angle between the spectra, treating them as vectors in a space with dimensionality equal to the number of bands. This technique, when used on calibrated reflectance data, is relatively insensitive to illumination and Aledo effects. SAM compares the angle between the end member spectrum vector and each pixel vector in n-dimensional space. Smaller angles represent closer matches to the reference spectrum. Pixels further away than the specified maximum angle threshold in radians are not classified.

2) Cross correlogram spectral matching (CCSM):

Cross correlogram spectral matching (CCSM) is a new approach towards mineral mapping from imaging spectrometer data. A cross correlogram is constructed by calculating the cross correlation at different match positions between a test spectrum (i.e., a remotely-sensed spectrum) and a reference spectrum (i.e., a laboratory mineral spectrum). To assess the sensitivity of the cross correlograms as a means of spectral matching, the technique is applied to laboratory spectra. In each experiment, the cross correlogram function was derived, a test of significance of the correlations was conducted and a moment of skewness was calculated to characterize the curve shape of the correlogram. The cross correlogram for a perfect spectral match had a parabolic shape with the maximum correlation of one at match position zero and a symmetry around the central match number. The cross correlation is found to be insensitive to differences in gain and thus allows to
compare materials of different albedos. The cross correlogram is relatively insensitive to noise which will reduce the overall correlation but does not affect the shape of the correlogram. Relative small differences in absorption band position and shape between the test and reference spectrum affect the shape, significance and correlation of the correlogram values.

3.1.3 Spectral Unmixing

Identification of the main constituents of the surface is only the first step in mapping using imaging spectrometer data because natural surfaces are rarely composed of a single uniform material. These surfaces are more commonly made up of mixtures or assemblages of intimately mixed minerals, alteration products, or weathered constituents [65-67]; and vegetation, water, and shadows. Spectral mixing is a consequence of the mixing of materials having different spectral properties within the ground field of-view (GFOV) of a single image pixel. Several researchers have investigated mixing scales and linearity. Singer and McCord (1979) found that if the scale of the mixing is large (macroscopic), then the mixing occurs in a linear fashion[68]. For microscopic or intimate mixtures, the mixing is generally nonlinear (Singer, 1981). Boardman addressed the macroscopic mixing problem using singular value matrix decomposition (SVD) to determine the scale of spatial mixing and to linearly unmixed AVIRIS data[69, 70]. This technique assumes that most mixing is on the macroscopic scale, and thus linear. For most situations, however, there is a significant amount of intimate mixing and therefore the linear unmixing techniques are at best an approximation. Abundances determined using these techniques are not as accurate as those determined using non-linear techniques, however, to the first order, they appear to adequately represent the surface conditions.

A spectral library of constituent spectra or "endmembers" typically forms the initial data matrix for the analysis. Ideally, these endmembers, when linearly combined should be able to match all possible spectra in the imaging spectrometer data. An inverse of the spectral library matrix is formed by multiplying together the transposes of the orthogonal matrices and the reciprocal values of the diagonal matrix. A simple vector-matrix multiplication between the inverse library matrix and an observed mixed image spectrum gives an estimate of the abundance of the library endmembers for the unknown spectrum. Data are typically first examined using unconstrained unmixing in which the derived abundances are free to take on any value including negative ones. The output of the unmixing processes an image data cube with the same spatial dimensions as the input data, with the "spectral" output bands representing the abundances of the endmembers. The analysis also usually produces two additional images, one showing the sum of the abundances at each pixel, and the other the root-mean square (rms) error values at each pixel. Interactive analysis of the abundance cube, the sum image, and the rms error image is used to determine if the endmembers explain most of the spectral variation. Subsequent inclusion of new endmembers and iteration are used until the rms error
is small and the results converge to non-negative values that sum to one or less (100%). Alternatively, fully constrained unmixing may be used, but this is much more computationnally intensive.

3.1.4 Spectral classification

Classification of a hyperspectral image sequence amounts to identifying which pixels contain various spectrally distinct materials that have been specified by the user. Several techniques for classification of multi/hyperspectral pixels have been used from minimum distance and maximum likelihood classifiers to correlation/matched filter-based approaches such as spectral signature matching and the spectral angle mapper. The statistically based classifiers are limited since they do not account for the prevalent case of mixed pixels which are pixels that contain multiple spectral classes. Existing correlation/matched filter-based approaches suffer from the mixed pixel problem, as well as the limitation that the output of the matched filter is non-zero and quite often large for multiple classes since the spectral signatures of materials are not generally orthogonal vectors. To reduce the data volume, techniques for reducing the image dimensionality are often applied. Typically, the dimensionality of a hyperspectral image cube is reduced by applying a linear transformation, such as a principal components transformation, and retaining only the significant components for further processing. The principal components transformation produces a new set of uncorrelated images that are ordered in terms of decreasing information or, equivalently, decreasing variance. Although each hyperspectral pixel is a high (>100) dimensional vector, most of the information about the scene can be described by a few (generally less than ten) dimensions. This reduced dimensionality is known as the intrinsic dimensionality. A recent improvement to the principal components transformation is the noise-adjusted principal components transformation. This transformation orders the new images in terms of signal-to-noise ratio, and thus overemphasizes noise in the resulting images. Although these approaches are sufficient for reducing data volume, they do not emphasize individual spectral classes or signatures of interest. For example, the first principal component image contains the most information/variance, but it is generally a linear combination of information from several spectral classes. This is a direct consequence of the fact that most materials resident in hyperspectral scenes have spectral signatures that are correlated, whereas the eigen vectors used to derive the principal component images are, of course, orthogonal.

3.1.5 Spectral feature extraction

Principal component analysis (PCA) is a mathematical procedure that uses an orthogonal transformation to convert a set of observations of possibly correlated variables into a set of values of linearly uncorrelated variables called principal
components. The number of principal components is less than or equal to the number of original variables. This transformation is defined in such a way that the first principal component has the largest possible variance (that is, accounts for as much of the variability in the data as possible), and each succeeding component in turn has the highest variance possible under the constraint that it be orthogonal to (i.e., uncorrelated with) the preceding components. Principal components are guaranteed to be unbiased only if the data set is jointly normally distributed. PCA is sensitive to the relative scaling of the original variables. Depending on the field of application, it is also named the discrete Karhunen Loève transform (KLT), the Hotelling transform or proper orthogonal decomposition (POD).

PCA was invented in 1901 by Karl Pearson. Now it is mostly used as a tool for exploratory data analysis and for making predictive models. PCA can be done by eigenvalue decomposition of a data covariance (or correlation) matrix or the singular value decomposition of a data matrix, usually after mean centering (and normalizing or using z-scores) the data matrix for each attribute. The results of a PCA are usually discussed in terms of component scores, sometimes called factor scores (the transformed variable values corresponding to a particular data point), and loadings (the weight by which each standardized original variable should be multiplied to get the component score).

PCA is the simplest of the true eigenvector-based multivariate analyses. Often, its operation can be thought of as revealing the internal structure of the data in a way that best explains the variance in the data. If a multivariate dataset is visualised as a set of coordinates in a high-dimensional data space (1 axis per variable), PCA can supply the user with a lower-dimensional data space picture, a "shadow" of this object when viewed from its (in some sense) most informative viewpoint. This is done by using only the first few principal components so that the dimensionality of the transformed data is reduced.

PCA is closely related to factor analysis. Factor analysis typically incorporates more domain specific assumptions about the underlying structure and solves eigenvectors of a slightly different matrix.
PCA of a multivariate Gaussian distribution centered at (1,3) with a standard deviation of 3 in roughly the (0.878, 0.478) direction and 1 in the orthogonal direction. The vectors shown are the eigenvectors of the covariance matrix scaled by the square root of the corresponding eigenvalue, and shifted so their tails are at the mean.

3.1.6 Endmember Extraction

The key task in linear spectral mixture analysis is to find an appropriate suite of pure spectral signatures (and), which are then used to model at-sensor pixel spectra through a linear combination of end member signatures. The selection outlandish can be performed in two ways: 1) by deriving them directly from the image (image end members) or 2) from field or laboratory spectra of known target materials (library end members); see for a comparison between the two. The risk in using library and is that these spectra are rarely acquired under the same conditions as the airborne data. Imageendmembers have the advantage of being collected at the same scale as the data and can, thus, be more easily associated with features on the scene.

A number of algorithms have been developed over the past decade to accomplish the task of finding appropriate image endometritis spectral mixture analysis [71]. It should be taken into account that the presence of pure class pixels in the image
data depends on available sensor spatial resolution. As a result, there may be cases where it is not possible for a certain algorithm to find such pure pixels in a scene. In those situations, the fractional components found for the mixed pixels are usually expressed in terms of other mixed pixels (the end members identified by the algorithm) and not in terms of pure classes. With the above statements in mind, and taking into account the increasing number crew member identification methods readily available, the need for standardized strategies to evaluate the quality of selected endmembers has been identified as a desired goal by the scientific community devoted to hyperspectral data analysis. Need the simplest evaluation approaches have been the comparison of end members with available ground-truth spectra. Spectral mixture analysis utilizes the high dimensionality of hyperspectral imagery to produce a suite of abundance fraction images for each end member. Each fraction map shows a sub-pixel estimate of end member relative abundance, as well as the spatial distribution of the end member. Therefore, the quality of a suite of endmembers can also be evaluated by looking at the spatial distribution of fractional abundances, i.e., by comparing estimated abundance fractions to exist ground-truth abundance maps. Comparative approaches mentioned above represent complementary strategies that can be applied to decide whether a method works correctly from two different points of view (spectral and spatial). However, these approaches are only possible when high-quality ground-truth information concerning the original scene is available. We must also consider that the generation of reliable ground-truth in real scenarios is difficult and expensive, a fact that has traditionally prevented the existence of comparative surveys using large databases of real images. In order to avoid this shortcoming, simulation of hyperspectral imagery has been suggested as a simple and intuitive way to perform a preliminary evaluation of analytical techniques. The primary reason for the use of simulated imagery as a complement to real data analysis is that all details of the simulated images are known. These details can be efficiently investigated because they can be manipulated individually and precisely. As a result, algorithm performance can be examined in a controlled manner.

3.2 Satellite images for Surface Mineralogy Mapping

Hyperspectral observations can provide information on material composition across whole geological systems. For example, a complete set of our information can be obtained over a large area to meet the needs of operational geological surveys. Countries around the world have realized the importance of hyperspectral remote sensing technology in exploration, fine mining, and many utilization, and hyperspectral mineral mapping technologies have been replicated widely.

Satellite and airborne hyperspectral payloads can obtain spectral data on the Earth's surface. Ground imaging spectrometers can obtain accurate hyperspectral information about rocks and minerals, and core spectral scanning systems can obtain data on underground rocks and minerals. Surface and subsurface stereo-mapping of
minerals based on these platforms has become a key research focus worldwide.

Data obtained by the hyperspectral imager Hyperion carried by the satellite EO-1, the thermal emission reflection radiometer ASTER carried by TERRA, the compact high-resolution imager CHRIS carried by PROBA, and the moderate-resolution imaging spectrometer MERIS carried by ENVISAT have been widely applied. In addition, Australia, Canada, Germany, France, Finland, Japan, and other countries have already been launched or are about to launch satellites equipped with hyperspectral imagers. Using hyperspectral satellite data, many researcher have achieved remarkable results in mineral exploration and resource utilization.

Some of China's relevant departments and research units have also used satellite-observed hyperspectral data for geological applications. Ganetal., for example, used Hyperion data to detect pollutants from the Dexing Copper mine[72]. The China Aero Geophysical Survey & Remote Sensing Center for Land and Resources (AGRS) also used Hyperion data to preliminaries identify some alteration minerals such as sericite (including high and low Al), kaolinite, and chlorite[73]. These studies all achieved good results.

Regarding airborne remote sensing, numerous countries have been working to develop airborne imaging spectrometers, among which the airborne visible and infrared imaging spectrometer (AVIRIS) and HyMap sensor are the most famous. Clark and Swayze used AVIRIS to obtain hyperspectral data for mapping cuprite in Nevada[74]. Suisse et al. Used AVIRIS images to compile maps of tremolite, actinolite, and talc[1]. Ellis used a HyMap sensor to obtain hyperspectral images and compile maps of kaolinite[75]. Levitical and Staenz extracted information on limestone and oxidized tailings from compact airborne spectrographic imager (CASI) images[76]. In 2007, the United States Geological Survey (USGS) used HyMap data covering all of the Afghan area for mineral exploration and hazard assessment in Afghanistan.

In China, there have also been many successful examples of aircraft acquisition of remote sensing data, especially in hyperspectral data. Based on my work in the Institute of Remote Sensing Applications, Chinese Academy of Sciences (IRSA, CAS), we distinguished Cambrian and Ordovician limestone from Permian limestone by mineral mapping using aviation imaging spectral data of the Tarim Basin, and identified lithostratigraphy according to separate rock spectral features. Extraction of alteration minerals was conducted and mineral mapping methods were tested using data obtained with a MASI sensor over the ZhangJiakou and Chongli-Chicheng areas of Hebei province, respectively. In addition also cooperated with Australia to use HyMap data to draw a 1:50000 scale map of alteration minerals and a 1:10000 scale map of abnormal mineral distributions.

For remote ground imaging and mineral exploration, portable shortwave-infrared instruments such as the portable infrared mineral analyzer (PIMA, Integrated
Spectronics Pvt Ltd., Australia) has been widely used. Chinese Geological Survey Development Research Center achieved good mapping results by establishing a PIMA prospecting model for the Xinjiang Tsuchiya porphyry mining area and the Yunnan Perlong porphyry copper mining area. In addition, I and my group have developed the field imaging spectrometer system (FISS), which has high spatial and spectral resolution and can be used for fine mineral classification and high-precision mapping.

3.2.1 Multi-spectral Images for Surface Mineralogy Mapping

3.2.1.1 ETM+

Geological investigation often adopts the ETM+ image to extract the construction and alteration information. ETM+ (Enhanced Thematic Mapper Plus) is the sensor in Landsat 7 by United States space agency NASA launched on April 15, 1999. The image can maintain the long-term continuous monitoring for global resource and environmental change. The sensor with 7 bands, from 0.45 μm to 2.35 μm, which covered the range of VIS and NIR. At the same time, the sensor carries a PAN band with 15m spatial resolution. The scale of the map can be up to 1:50,000 through the fusion method [77-80].

Using ETM+ to extract the geological information in China, it is already the general means same as geophysical, geochemical, geological means and so on. The project about nationwide mineral resources potential assessment use the ETM+ image to extract the construction, alteration, geological boundary, lithology information, and mapping scale to 1:50,000. The achievements about RS include RS imagery, RS alteration information extraction map, RS geological interpretation map. Whereas the limit of the image spectral resolution, it can extract the alteration information about Fe3+ (Fe2+) and OH-. Fe3+ information appears a little reflection peak in the 3th red band and an absorption valley in the first blue band. So often using the methods of (1) ratio to band3/band1, (2) PCA transformation to band 1, 3, 4, 5 to enhance the information of iron. The OH- information appears an obvious reflection peak in the 5th band and an absorption valley in the 7th band. So often using the methods of (1) ratio to band5/band7, (2) PCA transformation to band 1, 4, 5, 7, to enhance the OH- information. The alteration information can not be subdivided for details by limit to the spectral resolution.

3.2.1.2. ASTER

The ASTER instrument [81, 82], launched in December 1999, aboard the Terra satellite, is a cooperative effort between NASA, Japan’s Earth Remote Sensing Data Analysis Centre (ERSDAC), and Japan’s Ministry of International Trade and Industry (MITI). ASTER offers medium to high spatial resolution, a ground swath width of 60
km, and a revisit time of 16 days. The instrument is composed of three optical imaging subsystems acquiring fourteen multispectral bands operating in the visible near infrared (VNIR), shortwave infrared (SWIR), and thermal infrared (TIR) channels, each achieving spatial resolutions of 15 m, 30 m, and 90 m respectively.

ASTER offers substantial improvements over previous earth observation satellites such as the Landsat Thematic Mapper (TM), and Enhanced Thematic Mapper (ETM+) series. One improvement is seen in its thermal infrared capability, where ASTER offers 5 channels at a spatial resolution of 90 m (Table 1) - compared to TM and ETM+, which provide 1 channel at 120 m and 60 m respectively.

<table>
<thead>
<tr>
<th>Sub-system</th>
<th>Band number</th>
<th>Spectral range (µm)</th>
<th>Centre λ (µm)</th>
<th>Spatial resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>TIR</td>
<td>10</td>
<td>8.125 – 8.475</td>
<td>8.3</td>
<td>90 m</td>
</tr>
<tr>
<td></td>
<td>11</td>
<td>8.475 – 8.825</td>
<td>8.65</td>
<td></td>
</tr>
<tr>
<td></td>
<td>12</td>
<td>8.925 – 9.275</td>
<td>9.1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>13</td>
<td>10.25 – 10.95</td>
<td>10.6</td>
<td></td>
</tr>
<tr>
<td></td>
<td>14</td>
<td>10.95 – 11.65</td>
<td>11.3</td>
<td></td>
</tr>
</tbody>
</table>

• Table 1. ASTER TIR instrument characteristics

*Figure 3.4. Fully 70 km x 70 km image (SWIR -30 m resolution*
Figure 3.5. Zoom ~7.5km x ~7.5km (VNIR 15 m resolutions)

Figure 3.6. Remote Sensing Imagery of Tibet, China with ETM+ data (Tibetan geological investigation Academy, 2013)
ASTER remote sensing data for 1, 2, 3 and 4-band, Phyllosilicate minerals reflectivity with wavelength grows larger, halloysite only in 4-band with obvious absorption characteristics. Studies suggest using ASTER remotely sensed data can be extracted separately Al-OH groups and Mg-OH groups information. At the same time, the reflectivity of goethite and hematite in ASTER data bands 1, 2, 3, 4 with wavelength grows larger, and due to its reflectivity in band 3 is less than in band 4, to in 3 band formed a relative weaker of absorption peak. Jarosite in band 3 exists an obvious absorption peak, which is the spectral characteristic of Fe$^{3+}$. Comparasite analysis to ASTER and ETM+, the study indicated that ASTER data can extract the information of Fe$^{3+}$. The reflectivity of calcite minerals in band 1, 2 and 3 takes on an uptrend. CO$_3^{2-}$ in band 8 forms a distinct absorption peak, which is same as the absorption peak at 2.35μm [20].
3.2.2 Hyperspectral Images for Surface Mineralogy Mapping

3.2.2.1 Hyperion

NASA’s EO-1 Hyperion sensor, launched in November 2000, provides the first opportunity to evaluate short-wave-infrared (SWIR) spaceborne hyperspectral capabilities. Hyperion covers the 0.4 to 2.5 μm range with 242 spectral bands at approximately 10 nm spectral resolution and 30 m spatial resolution [10].

Spectroscopy in the solar spectral range, 0.4 to 2.5 μm, provides diagnostic information about many important earth-surface materials. In particular, the 2.0 to 2.5 μm (SWIR) spectral range covers vibrational features of hydroxyl-bearing minerals, sulfates, and carbonates common to many geologic units and hydrothermal alteration assemblages. “Hyperspectral” sensors or Imaging spectrometers provide a unique combination of both spatially contiguous spectra and spectrally contiguous images that allow mapping these features. Research-grade airborne hyperspectral data have been available for over 20 years and have proven the ability of these.

Systems to uniquely identify and map many minerals, even in sub-pixel abundances. The launch of NASA’s EO-1 Hyperion sensor in November 2000 marks the first operational test of a SWIR spaceborne hyperspectral sensor. Hyperodontidae 0.4 to 2.5 micrometer spectral range with 242 spectral bands at approximately 10 nm spectral resolution and 30 m spatial resolution over a 7.5 km swath from a 705 km orbit. Validation sites in a variety of geologic terrains were selected based on pre-existing abundant supporting information in the form of extensive field mapping and spectral measurements, and previous or scheduled airborne Hyperspectral data [83]. Results for selected sites in the USA and around the world have been previously reported.
3.2.2.2 TianGong

1) Introduction

Since Aerial Imaging spectrometer represented by AVIRIS obtained Hyperspectral data, hyperspectral remote sensing application in geology has been taken seriously [84]. Some typical Aerial Imaging Spectrometer, such as American AIS, HYDICE, SEBASS[13] and AVIRIS, Canada FLI, CASI and SFSI, Australian HyMap and Chinese OMISI[85], MAIS, as well as the space-borne hyperspectral imager, such as American Hyperion, ESA Chris, have get a large amount of Hyperspectral image data for geological applications.

Tiangong-1 is China's first target aircraft and space laboratory, which were launched at 21:16:03 on September 29, 2011 at the Jiuquan Satellite Launch Center. Chinese self-developed hyperspectral imager is one of the major remote sensing payloads which it carried. Compared to international existing satellite hyperspectral imager (such as EO-1 HYPERION and PROBA CHIRS), Tiangong-1 hyperspectral data have considerable advantages on the basic parameters in terms of wavelength range (covering the visible, near infrared and shortwave infrared), the number of bands or spatial resolution. Tiangong-1 hyperspectral imaging system is currently the highest spatial resolution and spectra composite indicator spatial spectral imaging system of China, which can realize imaging detection of nanosecond spectral resolution of terrain characteristics and properties.

Tiangong-1 hyperspectral imager data include hyperspectral imager panchromatic image, hyperspectral visible and near-infrared wave data (VNI), hyperspectral shortwave infrared wave data (SWI)[86]. The spectral range of Tiangong-1 hyperspectral visible and near-infrared wave data is approximately (0.4-1) μm, the Spectral resolution of which is about 10 nm and effective bands is more than 64. The spectral range Tiangong-1 hyperspectral shortwave infrared data was approximately (1.0-2.5) μm. The spectral resolution of which is approximately 23nm and effective wave bands is more than 64.

Hyperspectral data bank correlation detection method is a kind of hyperspectral data bank sequence structure analysis method based on Hyper-(Multi-) spectral background – abnormalities model [87]. Introspective advantages of structural analysis, anomaly detection, end-extraction, spectral matching and other alteration information extraction methods, alteration anomaly detection and extraction were done for Tiangong-1 hyperspectral data and then end member extraction and spectral matching was conducted.
2) Technical process

The alteration Information Extraction process of Hyperspectral band correlation detection is shown in Figure 3.10. Firstly, hyperspectral image correlation analysis is conducted to determine whether there exist alteration anomalies and select anomaly bands. Secondly, the anomaly image is output and masks the anomaly image by using a threshold. Thirdly, SMACC method is used to extract mineral and in the masked region of high anomalies and image atmospheric correction was required before end member extraction. Finally, by using SAM method, alteration mineral mapping is done on the basis of the standard spectral library.

![Figure 3.10. Alteration information extraction process of Hyperspectral band correlation detection](image)

2.1) Correlation Analysis

Hyperspectral image correlation analysis calculated the correlation coefficients of a set of continuous spectra bands and another set of continuous spectra bands. The correlation coefficients of a set of continuous spectra bands with a band in another set of continuous spectra bands on the graphic line segments similar to curve. The correlation coefficients of a set of continuous spectra bands with another set of continuous spectra bands on the graph are a series of approximate curves. This graph is called the correlation coefficient structure graph in this paper. The correlation coefficient structure graph of a set of continuous spectra bands near 2210 nm and another set of continuous spectra bands was calculated and if there exists concave features near 2210nm on the graph, the following steps is to be done.

2.2) Anomaly bands selections

Anomalopidae were selected based on the concave features on the correlation coefficient structure graph. There are three methods to select Anomaly bands. The first method is to select threes bands that are the left shoulder, right shoulder and
the lowest points of the concave feather weight X axis direction. The second way is a select band sequence that is the lowest point and both sides of the lowest point of the concave features in the x axis direction. The third method is to select two bands that formed the lowest point of the concave features called the band ordered pair.

2.3) anomaly output

In this paper, SAI Method [39] and PCA method was used to output anomalies. SAI method was applied to the first anomaly bands selection method. PCA applications can apply to both the second and the third anomaly bands selection method.

2.4) Endmember extraction and spectral mapping

Masked region of the extraordinary anomalies is created from the anomaly image. To extract mineral end members in masked region of high anomalies and the image atmospheric correction is required before endmember extraction. This paper uses the sequential maximum angle convex cone method (SMACC). Using spectral angle mapping method to do mineral mapping by the mineralogists of standard spectral library corresponding with the extracted endmember spectral.

3) Results

![Figure 3.11. Alteration mineral mapping](image)

(a) Low Al sericite mineral (b) High Al sericite mineral (c) Kaolinite mineral (d) Chlorite mineral
3.3 Airborne hyperspectral images for Surface Mineralogy Mapping

3.3.1 Aviris

The Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) was the first imaging sensor to measure the solar reflected spectrum from 400 nm to 2500 nm at 10 nm intervals [16]. The calibration accuracy and signal-to-noise of AVIRIS remain unique. The AVIRIS system as well as the scientific research and applications has evolved significantly in recent years. The AVIRIS system was designed, developed, upgraded, and maintained to support a range of NASA research and applications objectives. The initial design of the sensor with an efficiencies mirror, f/1 spectrometers, and 200 lm detectors has enabled a series of upgrades that resulted in high signal throughput and low noise performance. A parallel set of upgrades has focused on stabilizing the spectrometers and onboard calibrator as well as developing a set of new spectral, radiometric, and spatial calibration techniques. In combination, these efforts resulted in the current accurate spectral, radiometric and spatial calibration as well as high signal-to-noise of AVIRIS. With the increased demand for AVIRIS spectral images, the data system was upgraded to take advantage of new computer and mass storage technology. This upgrade also resulted in the breakup of the monolithic AVIRIS processing program into a series of simple program modules dedicated to the calibration and distribution of each year’s data. As the sensor, calibration and data system evolved, the flight operations procedures and technology were improved. The AVIRIS system acquires the research and application data sets requested by the investigator and that the AVIRIS sensor is performing nominally before, during, and after each flight. Both e-mail and the AVIRIS website now play an important role in keeping investigators informed of acquisition and performance status. The upgrades to the sensor, calibration, data system, and flight operations leave AVIRIS in a strong position to continue to support research and applications in the future.
3.3.2 Hymap

Kip, an advanced hyperspectral sensor developed by Integrated Spectronics, Sydney Australia, represents the current state-of-the-art in airborne hyperspectral remote sensing (Figure 3.14). Han data can map environmental surface features such as contaminated vegetation, acid mine drainage, buffering minerals, features of vegetation stress and a few types of water suspensions.
Hyperspectral Mapper (HyMap) has been developed in Australia and deployed for commercial operations around the world in 1997. It was delivered as a 96 channel instruments operating over the wavelength range 0.55 – 2.5 um. Then Subsequent HyMap sensors have been delivered with up to 128 bands covering the 0.44 – 2.5 um spectral region and with two thermal bands (one band in the 3 – 5 um atmospheric window and another in the 8 – 10 um spectral region). This type of configuration is now finding an expanding role in tasks such as environmental pollution monitoring, agriculture and forestry, soil mapping and the assessment of natural and introduced vegetation. It is one of the few hyperspectral sensors that has been commercially deployed, and is thus the subject of a great deal of research in the earth observation field at present. This sensor had been used to estimate the abundance of smectite at Tudun mining area of Xinjiang Province, China.

Figure 3.14. The HyMap sensor

Figure 3.15. abundance of smectite is estimated from HyMap data at Tudun mining area of Xinjiang
3.3.3 CASI

The Compact Airborne Spectrographic Imager (CASI), Canadian hyperspectral airborne instrument, is a commercially available sensor operating in the visible and near-infrared (VNIR) from 400nm to 1000nm. A f/4 reflection-grating spectrograph is coupled to a CCD (charge coupled device) sensor, providing a resolution of 578 spatial pixels; the spectrum from 450 nm-950 nm for each spatial pixel is dispersed across 288 spectral pixels. CNNC Beijing Research Institute of Uranium Geology import CASI in 2008 and took a research and distribute of rocks being rich in Fe$^{2+}$ and the abnormal area of uranium.

![Figure 3.16. Distributing of rocks being rich in Fe$^{2+}$ (red color area) and the abnormal area of uranium (in the circularity) using CASI data](image)

3.4 Field hyperspectral images for Surface Mineralogy Mapping

3.4.1 HySpex SWIR-320m

One ground based hyperspectral sensor that has recently been developed is the HySpex SWIR-320m by NorskElektroOptikk AS, Norway. This sensor operates in the short wave infra-red (SWIR) part of the electromagnetic spectrum, from 1.3-2.5um, giving the required range for detecting absorption bands in common minerals such as carbonates and siliciclastics. Particularly, carbonate minerals are well-suited to the SWIR sensor after study by a number of authors [88-91]. The seminal publication by
Hunt and Salisbury (1971) [88] presents the spectral curves and absorption features found in carbonate minerals. Geffey (1986) [90] found at least seven carbonate absorption bands in the 1.6-2.5 unspecified range due to vibration processes of the carbonate ion, and indicates the position and the shapes of these bands as diagnostic features to identify the rock forming minerals calcite, aragonite and dolomite. Van der Meer (1995) [91] shows that calcite and dolomite from the two end-members of a continuous series with a linear mixture relationship. He concludes that the shape and the exact position of the absorption feature in the 2.3-2.4 um spectral range may be used to predict the relative abundance of calcite and dolomite in a rock sample. Van der Meer (1996) [67] demonstrates the mapping of carbonate lithofacies from Landsat TM data using spectral mixture models.

<table>
<thead>
<tr>
<th>Detector</th>
<th>CT (HgCdTe)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral range</td>
<td>1.3-2.5 mm</td>
</tr>
<tr>
<td>Spatial pixels</td>
<td>320</td>
</tr>
<tr>
<td>Field of view across track</td>
<td>14°</td>
</tr>
<tr>
<td>Pixel field of view</td>
<td>~0.75 mrad</td>
</tr>
<tr>
<td>Spectral sampling</td>
<td>5 nm</td>
</tr>
<tr>
<td>Spectral bands</td>
<td>256</td>
</tr>
<tr>
<td>Digitization</td>
<td>14 bit</td>
</tr>
</tbody>
</table>

*Table 2. Key characteristics of HySpex SWIR-320m sensor*

Figure 3.17 shows the HySpex SWIR-320m sensor in the field. Though it is still a newly developed instrument and not yet fully field “ruggedized”, the system is portable enough for field use, and is similar in components to a terrestrial laser scanner, whilst weighing slightly less. The ease of use and portability is critical aspects for geological outcrop work. Airfield sites are often in remote areas and not always close to roads. With 320 spatial pixels, the hyperspectral sensor is much lower resolution than a contemporary digital camera; however, resolution is sure to increase in the future as it did for CCD/CMOS sensors. For this pilot project, geological problems to be targeted must take into account the scale of features to be studied, as well as the available spatial resolution. The advantage of the HySpex sensor is that it offers superior spectral resolution (Table 1). Integration of the hyperspectral data with lidar and visible images a complementary approach to obtain high spatial and spectral coverage of the outcrop.
3.4.2 PIMA

The PIMA (Portable Infrared Mineral Analyzer) is a field spectrometer equipped with an internal illumination source powered by a 6-V rechargeable battery. The spectrometer weights around 3kg. Insenses hemispherical reflectance in 601 spectral channels across the SWIR region from 1,300 to 2,500 nm, with 2-nm spacing between the centers of adjacent spectral channels. This instrument is fully calibrated against a built-in wavelength standard, composed of several natural minerals and synthetic materials with sharp SWIR absorption features. Spectral data acquisition are rapid, taking about 20–60 s. Sample preparation is not required and spectra can be acquired from drill-core, rock chip and powder. Thus, it is practical to measure a large number of samples to capture the details of mineralogical variation in drill-holes, trenches, and throughout an entire altered and mineralized system.

The PIMA-II measures hemispherical reflectance of samples in 601 spectral channels across the wavelength region from 1.3 to 2.5 mm. This instrument is calibrated against wavelength and reflectance standards. The spectrometer weights around 3kg. It operates with an internal illumination source and is powered in the field by a 6-V rechargeable battery. As the overtone sand combination tones of the OH⁻, SO₄²⁻ and CO₃²⁻ groups are prominent in the SWIR [29, 88], the PIMA-II is particularly useful for identifying sheet silicates, sulfates and carbonates. It takes about 30±60 s to collect a spectrum. Samples to be measured can be in the form of core. Rock chip, cutting or powder, without any preparation procedure required. Thanatos, the rapid spectral collection and non-sample preparation, it is practical to measure with a PIMA II a large number of samples to capture details of the mineralogical variations down a single drill-hole or, indeed, throughout the explored part of a geothermal system.
3.5 Mineral mappings at the northern Death Valley

Imaging Spectrometers, or “hyperspectral” sensors provide a unique combination of both spatially contiguous spectra and practically contiguous images of the Earth’s surface unavailable from other sources. Research-grade airborne hyperspectral data have been available for over 20 years. Current airborne sensors provide high spatial resolution (2–20 m), high-spectral resolution (10–20 nm), and high SNR (500 : 1) data for a variety of scientific disciplines.

The Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) represents the current state of the art. AVIRIS, flown by NASA/Jet Propulsion Laboratory (JPL) is a 224 channel imaging spectrometer with approximately 10nm spectral resolution covering the 0.4–2.5m spectral range [46]. The sensor is whisk broom system utilizing scanning fibreoptics to acquirecross-track data. The IFOV is 1 rad. Four off-axis double-pass Schmidt spectrometers receive incoming illumination from trophotropic using optical fibers. Four linear arrays, one for eachspectrometer, provide high sensitivity in the 0.4–0.7, 0.7–1.2,1.2–1.8, and 1.8–2.5 umbrageous, respectively. AVIRIS is flown as a research instrument on the NASA ER-2 aircraft at an altitude of approximately 20km, resulting in approximately 20-m pixels and a 10.5-km swath width. Since 1998, it has also been flown on a Twin Otter aircraft at low altitude, yielding 2–4-m spatial resolution.

3.5.1 Method

AIG has developed methods for analysis of hyperspectral data that allow reproducible results with minimal subjective analysis (Figure 3.36). These approaches are implemented and documented within the “Environment for Visualizing Images” (ENVI) software system originally developed by AIG scientists (now an Eastman Kodak/Research Systems Inc. (RSI) commercial-off-the-shelf (COTS) product). The Hyperspectral analysis methodology includes the following:

1) Data preprocessing (as required);
2) Correction of data to apparent reflectance using the atmospheric correction software;
3) Linear transformation of the reflectance data to minimize noise and determine data dimensionality;
4) Location of the most spectrally pure pixels;
5) Extraction and automated identification of endmember spectra;
6) Spatial mapping and abundance estimates for a specific and.

A key point of this methodology is the reduction of data in both the spectral and spatial dimensions to locate, characterize, and identify a few key spectra (end members) that can be used to explain the rest of the hyperspectral dataset. Once
these endorsements selected, then their location and abundances can be mapped from the linearly transformed or original data. Thermometer derive the maximum information from the hyperspectral data themselves, minimizing the reliance on a priori or outside information.

1) Destriping for Hyperion Area Array Data: If required, preprocessing/data clean up may be applied to the data prior to atmospheric correction. In the case of Hyperion data, though radiometric corrections were applied prior to data delivery to AIG, there was still a pronounced vertical striping pattern in the data (visible in individual bands, but more pronounced when using the linearly transformed data). Such striping is often seen in data acquired using pushbroom (area array) technology (e.g. Airborne Imaging Spectrometer (AIS), Hyperion) and may be caused by factors such as detector non linearities, movement of the slit with respect to the focal plane, and temperature effects. Previous describing efforts suggest that a simple dark current (DC) imbalance (DC bias) of the detectors across the pixel direction of the detector array may explain the striping, and simple per-column DC offset is sufficient to correct the problem.

Description of the Hyperion data was accomplished using custom software (following the model of software written for the original push broom imaging spectrometer (AIS)). This approach adjusts each image column brightness (in all bands) based on a calculated offset relative to the scene average detector response. Assumptions made were that individual detectors were reasonably well behaved (stable) and that over the course of a data collect (“flightline”), that each of the cross-track detectors has covered, on the average, very similar surface materials (this second assumption is usually valid in desert environments, but may not be for other, more complex scenes). Implementation consisted of calculation of an average spectrum (242 bands) for each of the 256 Hyperion detectors followed by determination of a global scene average spectrum. Each column spectrum was then subtracted from the global spectrum to determine offsets to be added to each pixel in the corresponding column. Each pixel in each column of the radiance data was then adjusted accordingly using the calculated offset. This description is only required for correcting thoroughbred Hyperion data, and thus no describing was applied to the AVIRIS data.
2) Atmospheric Correction: Our analysis methods are generally applicable to both airborne and satellite data; however, the methodology requires processing radiance-calibrated data to apparent reflectance. Atmospheric correction Now (ACORN), currently used for correction of both airborne and satellite hyperspectral data, is commercially available enhanced atmospheric model-based software that uses licensed MODTRAN4 technology to produce high-quality surface reflectance without ground measurements. AVIRIS and Hyperion data were both converted to apparent reflectance using ACORN. Appropriate model parameters for each instrument (e.g., sensor altitude), collection date (e.g., date, time, seasonal atmospheric model), and location (e.g., latitude/longitude, average elevation) were used; otherwise, all other parameters were identical for both datasets.

3) AIG-Developed Hyperspectral Analysis: AIG-developed hyperspectral analysis methods used for both the airborne sensors and Hyperion data (implemented in the ENVI image analysis software) include spectral polishing, spectral data reduction using the MNF transformation, spatial data reduction using the Pixel Purity Index (PPI), an n-Dimensional Visualizer to determine image end members, identification of end members using their reflectance spectra in the Spectral Analyst, and mineral mapping using both the Spectral Angle Mapper (SAM), and Mixture-Tuned Matched Filtering (MTMF). This approach is shown in Figure 3.18.

4) Geometric Corrections: The final step in the analysis is usually to present the results on a map base. In this case, to facilitate comparison of Hyperion data to AVIRIS mineral-mapping results and minimize resampling artifacts, the AVIRIS data were used as the base rather than a map. The Hyperion data were
geometrically corrected to match the AVIRIS data for packing house control points (GCPs) and using a first-degree polyphonically with nearest neighbor resampling. Approximately 20GCPs were used, and the residual errors were on the order of two pixels. Hyperion image maps (not the full data cube!) were geocorrected to match the AVIRIS data.

3.5.2 Mapping Results

Operationally, spectral bands covering the shortwave infrared spectral range (2.0–2.4 m) were selected, and these bands were linearly transformed using the MNF transformation. Figure 3.19 shows plots of the MNF eigenvalues for the two datasets. Higher eigenvalues generally indicate higher information content. The MNF results indicate that, for both cases, the AVIRIS data contain significantly more information than the Hyperion data covering approximately the same spatial area and spectral range. The actual data dimensionality is usually determined by comparing both the eigenvalue plots and the MNF images for each dataset (Figures 3.19–23). In the case of the Cuprite AVIRIS, the MNF analysis indicates a dimensionality of approximately 20. The Cuprite Hyperion data exhibits dimensionality of approximately six. For the northern Death Valley site, AVIRIS shows dimensionality of approximately 20 and Hyperion roughly eight.

![Figure 3.19. MNF Eigenvalue plots for (left) the Cuprite, NV and (right) northern Death Valley, California and Nevada. AVIRIS and Hyperion data.](image)

![Figure 3.20. MNF images for Cuprite AVIRIS SWIR data. (Left to right) MNF band 1, MNF and 5, MNF and 10, MNF and 20.](image)
Figure 3.21. MNF images for Cuprite Hyperion SWIR data. (Left to right) MNF band 1, MNF and 5, MNF and 10, MNF and 20.

Figure 3.22. MNF images for northern Death Valley AVIRIS SWIR data. (Left to right) MNF band 1, MNF band 5, MNF band 8, MNF and 10, MNF band 20.
The top MNF bands for each dataset (analogous to the approximate dimensionality), which contain most of the spectral information, were used to determine the most likely endmembers using the PPI procedure. These potential endmember spectra were then loaded into a n-dimensional (-D) scatter plot and rotated in real time on the computer screen until “points” or extremities on the scatter plot were exposed. These projections were “painted” using region-of-interest (ROI) definition procedures and then rotated again in three or more dimensions (three or more MNF bands) to determine if their signatures were unique in the MNF data. While this portion of the analysis presents the greatest opportunity for subjective bias, iterative -D rotation and examination of remaining data dimensionality after selection of each subsequent endmember minimizes this effect and maximises the chance of reproducible results. Additionally, “class collapsing,” which rotates selected endmembers to a common projection and enhances remaining endmember locations in the scatter plots, allows an analyst to determine when all of the inherent and have been located.

Once a set of unique pixels was defined using the -D analysis technique, then each separate projection on the scatter plot (corresponding to a pure end member) was exported to a ROI in the image. Mean spectra were then extracted for each ROI.

From the apparent reflectance data, to act as end members for spectral mapping for both the Cuprite site (Figure 3.24) and the northern Death Valley site (Figure 3.25). These end members or subset of these end members (in the case of AVIRIS) were
used for subsequent classification and other processing. MTMF, a spectral matching method, was used to produce image maps showing the distribution and abundance of selected minerals (Note: MNF end member spectra, not reflectance spectra, aroused in the MTMF). The results are generally presented either as gray scale images with values from 0.0 to 1.0 (not shown), which provide a means of estimating mineral abundance, or as color mineral maps showing the spectrally predominant material for each pixel (Figures. 3.26–28). Basic mineral mapping was performed for the Cuprite site (Figure 3.26). Two image maps were produced for the northern Death Valley site, and first, a detailed mineral map showing minerals and mineral variability (Figure 3.24) an

Figure 3.24. Comparison of selected (left) AVIRIS end member spectra and (right) Hyperion end member spectra for the Cuprite, NV site. Note that AVIRIS detected several varieties of alunite plus an additional kaolinite-group mineral (dickite) that were not detectable using the Hyperion data.
Figure 3.25. Comparison of selected (left) AVIRIS end member (mean) spectra and (right) Hyperion end member (mean) spectra for the northern Death Valley, California and Nevada site.

Figure 3.26. MTMF mineral maps for (left) AVIRIS and (right) Hyperion produced for the end members in Figure 3.24 for the Cuprite, NV site. Colored pixels show the spectrally predominant mineral at concentrations greater than 10%.
Figure 3.27. MTMF mineral maps for (left) AVIRIS and (right) Hyperion produced for the end members in Figure 3.25 for the northern Death Valley, California and Nevada site. Colored pixels show the spectrally predominant mineral at concentrations greater than 10%.

Figure 3.28. MTMF mineral maps for (left) AVIRIS and (right) Hyperion produced a subset of the end members in
3.5.3 Discussion

Visual comparison of the AVIRIS and Hyperion mineral maps of both sites shows that Hyperion generally identifies similar minerals and produces similar mineral-mapping results to AVIRIS. Our results indicate, however, that the lower SNR of the Hyperion data do affect the ability to extract characteristic spectra and identify individual minerals (Figures 3.24–27). Specifically, compare the Hyperion benediction spectrum in Figure 3.24, which does not clearly show the characteristic budding tonite spectral feature shape near 2.11um, to the well-resolved feature extracted from AVIRIS (Figure 3.24) and other hyperspectral aircraft data. Note that while it generally appears that the difference in pixel size (30 m for Hyperion versus approximately 16 m for AVIRIS) is minimal (causing only slight loss of spatial detail in Hyperion results), some of the spectral difference could be an effect of the pixel size, causing greater mixing in the Hyperion data for relatively small benediction occurrences. Other examples of the limitations of Hyperion imposed by lower SNR than AVIRIS include the inability to separate mineral variability such as that caused by cation substitution (K versus Na influences, and Al versus Fe substitution in mica) and crystal structure differences (kaolinite versus dickite) at SNR less than approximately 50 : 1 (Figures 3.24 and 3.26). Our analysis indicates that the Cuprite Hyperion data do not allow extraction of the same level of detailed mineralogical information as AVIRIS. Figure 3.26 shows only a basic AVIRIS mineral map. Other researchers have demonstrated mapping of other minerals using AVIRIS at the Cuprite site that was not detected using the March 2001 Hyperion data. Finally, determination of abundances for minerals identified by AVIRIS and Hyperion is possible, but not illustrated here. Actually, Hyperion performs quite well considering the overall SWIR SNR.
Chapter 4 Mapping drill cores using imaging spectrometry

Imaging spectrometry, simultaneous measurement of continuous spectra and images in up to hundreds of spectral channels or bands, is a proven technology for identifying and mapping minerals based on their reflectance or emissivity signatures [92-94]. It has also become known as ‘hyperspectral imagery’ or ‘HSI’. Imaging spectrometry’s unique nature for remote mapping of surface materials relies on its capability to identify materials based on their electronic molecular spectral signatures in the visible and near-infrared (VNIR) and their vibrational molecular spectral signatures in the short-wave IR (SWIR) and long-wave IR (LWIR) spectral ranges. Mineral mapping using imaging spectrometer data is well established and routinely used for numerous geologic applications. In addition to typical airborne and satellite hyperspectral data acquisitions, spectroscopy has also been used in a limited way for analysis of drill cores and for outcrop scanning. More recently, concentrated efforts have been directed at operational spectral logging of drill cores using automated methods. Core imaging efforts are, however, still in the early stages of development [19].

This research describes an approach to and results from analysis of groups of field spectra using "hyperspectral" image processing techniques that provides a cost effective, quantitative measure of core composition. This methodology is an obvious extension of previous work done using multispectral scanner data to provide images for improved digital and photo interpretive extraction of geologic information from slabs of cores. In the following section, the research progress of mapping of minerals in drill cores will be introduced from three aspects: data collection system, data analysis methods and typical applications.

4.1 The instrument of FISS

The Field Imaging Spectrometer System (FISS) is the first imaging sensor aimed specifically at field imaging spectrometer in China [95] [96, 97]. Fig. 1 shows a schematic diagram of the FISS; utilizing a 464 × 344 CCD chip, it measures incoming radiation in 344 contiguous spectral channels in the 437–902-nm wavelength range with spectral resolution of better than 5 nm, and it creates images of 464 pixels for a line of targets with an instantaneous field of view (IFOV) of ~1 mrad. Specifically, the second spatial dimension of the sensor is accomplished by a scan mirror whose field of view and speed can be easily adjusted through the operating software. This means that there is no need to move FISS forward to image a wide range of targets.
Figure 4.1 shows a photograph of the FISS optical mechanical subsystem: from upper left to lower right of the enclosed optical mechanical subsystem are the CCD camera, which is built with area array detectors and a cooling device, the dispersing unit with a “prism-grating-prism” (PGP) element, the objective lens, and the scan mirror. The latter is attached to a stepper motor.

The FISS is a compact high-performance versatile instrument for a multitude of imaging spectroscopy applications, ranging from field use to laboratory and industrial use. The advantages of FISS were confirmed in our preliminary calibrations and applications. To facilitate imaging spectral measurements, the FISS is designed with many optional system settings that can be manually adjusted through the operating software or the optical mechanical head (Fig. 2) of the FISS [96, 97, 99]. It focused on improvement or redesign of the imaging system, optical splitting system, and control software. The imaging system is similar to that of PHI; the direction along the slit forms a spatial line image, while that perpendicular to the slit measures the spectrum for each line pixel made by the dispersion component [96, 100, 101]. A second spatial dimension is covered by the scanning mirror.
4.2 The instrument of SWIR FISS

A SWIR hyperspectral imaging system consisting of a XEVA-FPA-2.5-320 detector and a N25E spectrometer from Specim Corporation is set up to measure spectral range 1 to 2.5 µm, meaning that the interesting wavelengths from 0.4 to 2.5 µm can be covered by two FISS system.

Figure 4.3 descripted the optical and mechanical structure of SWIR system that covers 1000-2500nm wavelength range, with 30µm slit and corresponding 8-12nm spectral resolution. From left to right are detector, spectrometer, and scanning mirror. A solid ring is fixed on the spectrometer with a M6 screw fixed onto a holder. The scanning mirror is controlled by a step motor, swing from one side to another,
reflecting diffuse reflection light of sample to imaging lens. Then light is focused onto the entrance slit of spectrometer, which is based on the Prism-Grating-Prism (PGP) principles produced of Specim corporation, as commonly used in hyperspectral imaging system. The entrance slit here is used as a stop that only allows a narrow line of the scene to pass through. Grating in the PGP is designed to operate at Bragg condition and the angles of prism changes accordingly. Collimated light dispersed through the PGP along the optical axis, so that the central wavelength light pass axially, with shorter and longer wavelength dispersed symmetrically[102]. Figure 4.4 describes the optical principle of PGP imaging spectrometer.

Dispersed light is then focused onto MCT detector by another focusing lens in the spectrometer, locating behind the PGP. SWIR detector is sensitive to temperature change. So HgCdTe detector and control and communication electronics are all packed in one compact house. Four stage thermo-electrically cool methods are used to cool the entire house. As a whole the instrument will perform high spatial and spectral resolution, high signal-to-noise (SNR) with low stray light.

With SWIR spectrometer we measured spectrum of the stone samples indoor, and compared the result with measurement of PSR (PSR3500, Spectral Evolution). A halogen lamp is used to illuminate the stone and diffuse reflectance standard uniformly, and a data cube is acquired with background subtracted. Figure 4.5 shows the measured spectrum result.
4.3 Core drill imaging spectrometry system design

A wide variety of VNIR and SWIR airborne imaging spectrometers have been or are currently being flown. Here we focus on introducing a few typical representatives.

(a) ProSpecTIR-VS scanner

The ProSpecTIR-VS hyperspectral system operated by SpecTIR and LLC is a custom-integrated system that incorporates Specim’s Airborne Imaging Spectrometer for Applications (AISA), Eagle (VNIR) and Hawk (SWIR) imaging spectrometers. The combination of these two high-performance sensors provides for the simultaneous acquisition of full hyperspectral data covering the 0.4–2.45 μm spectral range. The two imaging spectrometers are co-aligned and generate a single, full-spectrum data cube covering 320 pixels cross-track. In airborne operation, as a pushbroom instrument and utilizing a 24° scan and 0.075° (approximately 1.3 mrad) instantaneous field of view (IFOV), the system achieves spatial resolutions varying from 0.5 to 5 m depending upon altitude and platform speed. The data collected for this experiment constitute spectral measurements in 360 spectral bands in total, covering the 0.4–2.45 μm spectral range at approximately 5 nm spectral resolution. The ProSpecTIR-VS sensor was operated in three different modes for the purposes of this research: (1) airborne over flight data at approximately 1 m spatial resolution, (2) core and rock-chip scans using a custom scanning bed and artificial (halogen) illumination at approximately 2 mm spatial resolution and (3) mine-wall scans using a truck-mounted scanning configuration and solar illumination at approximately 4 cm spatial resolution.

The ProSpecTIR-VS system was installed in a custom laboratory configuration to allow scanning of rock cores and rock chips, heretofore referred to as ‘core’. The setup consists of a sensor mount, scanning bed, artificial illumination and computer
control module. Twenty-three core boxes and seven rock-chip trays were run sequentially through the imaging spectrometer at a distance of about 1 m under artificial (halogen) illumination. The raw spectral data were converted to radiance using the same methods as for the airborne imagery described above, providing high signal-to-noise data across the entire spectral range of the imager. A large Spectrum on reflectance reference panel was run periodically with the core to allow correction to reflectance using a flat-field approach (dividing each pixel spectrum by the average Spectrum on spectrum). This correction to Spectrum on reflectance was done column by column due to the variation in cross-track lighting provided by the prototype system shown in the figure. Combined VNIR/SWIR test scans (∼360 bands 0.4–2.45 μm) and several SWIR-only (236 bands, 0.98–2.45 μm) scans were performed.

(b) HyLogging™ systems

CSIRO’s prototype HyLogging™ systems are integrated hardware and software systems that facilitate the rapid collection of high-density spectral reflectance measurements and continuous high-resolution color imagery of drill core/chips/powders. HyLogging is non-destructive and the core/chips are measured in their original trays. The robotically controlled procedure, coupled with the largely automated processing software, The Spectral Geologist (TSG) - Core, enables the identification of a suite of minerals by their diagnostic spectral absorption features displayed in the Visible-to-Near-Infrared (VNIR) to Short-Wave-Infrared (SWIR) regions and the Thermal Infrared (TIR) region of the electromagnetic spectrum.

HyChips™ is a part of CSIRO’s range of HyLogging™ tools. HyLogging™ tools are based on reflectance spectroscopy, which determines diagnostic spectral features caused by molecular vibrations indicative of the chemical bonds in selected crystalline minerals. HyChips™ systems are modular and a basic system typically comprises:

1) Integrated visible, near and shortwave infrared spectrometers covering the 400 to 2500 nanometer spectral range (that is, 0.4 to 2.5 micrometers);
2) a robotic x/y table for moving samples in their original containers beneath the spectrometers;
3) a digital camera capable of 0.2 mm resolution;
4) a laser profilometer for determining sample height or core breaks;
5) a control software.
The standard field-of-view (FOV) of the spectrometer is ~10mm. Its spectral and spatial sampling rate can be varied to ensure a high signal-to-noise ratio combined with high throughput. HyChips™ includes a device to remove or minimize wavelength breaks between spectrometers thus increasing data quality. HyChips™ instruments can be configured in three sizes suitable for one, three or six chip trays and are designated HyChips-1, HyChips-3 and HyChips-6 respectively. HyChips-1 is a potential small desk-top instrument, while HyChips-3 and -6 have been configured as table or floor mounted units. Floor-mounted HyChips-6 units can be used for low-volume core logging. High-volume core logging is better conducted using the HyLogger™.

The HyLogging™ technology allows collection and manipulation of large sample populations, and three-dimensional and data rich information sets. These data sets can be applied to a number of disciplines within different industries:

1) Mineral and petroleum exploration

HyLogging™ technology supports exploration geologists by providing improved geological data acquisition and interpretation productivity. It ensures maximum benefits from expensive drilling programs.

2) Mining and geotechnical

The HyLogging™ technology has realized applications in the production-mine situation. The extensive information available to technical personnel allows better understanding of the geotechnical properties and mineral associations of the ore system. With improved ore models more effective mining strategies can be developed, and grade control optimized, to potentially reduce operational costs.
3) Mineral processing

The field of geometallurgy is becoming increasingly important as mining companies are forced to invest in ores previously considered unviable due to processing difficulties and costs. Geometallurgy utilizes knowledge of the mineralogy and mineral chemistry of an ore system to select and model potential processing strategies. An understanding of the ore system can provide information about grind ability, reagent selection, ore blending options and the presence of deleterious minerals that may consume reagents or pose material handling issues.

There is also the potential for HyLogging™ technology to be used in an ‘in-stream’ capacity to monitor the mineral components of the ore as it enters the processing plant.

4.4 Jiama 3D mapping

BJKF instrument was produced by Nanjing Zhongdi instrument co. Ltd, China. The instrument with 3 types developed from wired data communication to Bluetooth data transmission. It is used to identify the silicate minerals containing (1) OH-, Epidote, and amphibole and so on, (2) sulphate minerals, e.g. alunite, jarosite, gypsum and so on, (3) carbonate minerals, e.g. calcite, and dolomite and so on.

The instrument is mainly applied to geological analysis, including: (1) qualitative and semi-quantitative mineral identification, (2) characteristics of mineralizing environment description, (3) original rock identification, (4) mineralization relationship indication, (5) weathering range and process indication, (6) chemical process of mineralization indication, (7) alteration minerals mapping.
The instrument was experienced we cooperated Chengdu University of Technology in Jiamacopper-polymetallic ore deposit, Tibet. Through the measurement of 5862 rock samples, it is evidenced the value of the instrument in geology. Rock spectral measurements in Jiama involve 20 km$^2$ region-wide and find most areas are covered by crystalline limestone with non-alteration characteristic. At the same time, some alteration rock mainly includes muscovite white mica, chlorite, kaolinite, dickite, ankerite, calcite, biote, and hornblende and so on. Through the study of the distribution of the alteration rock, it is found the potential for prospect nearby the Jiama ore. The finding enlarges the scale of the deposit, increases the reserves of ore-body further and brings the huge profit for the development corporation.
Figure 4.9 Quantitates computations about the mixed minerals complexity measured by BJKF instrument

Figure 4.10 The relationship of white mica measured by BJKF and contents of the same rock sample
Chapter 5 Conclusions and Recommendation

5.1 Conclusions

According to China’s national strategy, China will strengthen technological and application innovations, improve mineral resource detection by spaceborne and airborne hyperspectral remote sensing, establish platforms for ground-spectra measurement and drill-core scanning, compilation, and analysis, and develop data integration of astronomic, aerial, surficial, and below-ground remote sensing detection.

In this report, we introduced how to use satellite, aerial, surficial, and subsurface detection methods to capture object spectral data and establish a mineral resources spectral database. In the near future, we will develop technology for efficiently detecting mineral and energy resources, establish a sound platform for mineral resource and energy surveys, provide an operational system to meet the needs of resource developers, and construct a business model for integrated mineral and energy exploration with reasonable allocation of resources.

The goal of this report is to analyze the research status of hyperspectral remote sensing technology and restricting factors in mineral exploration applications, research key hyperspectral technologies and equipment for satellite, aerial, surficial, and subsurface observations, establish a preliminary global satellite hyperspectral data management system, improve and integrate aerial hyperspectral remote sensing systems based on existing imaging equipment, develop shortwave infrared field imaging spectrometers for rapid mineral mapping, and develop an efficient core analysis and logging system to retrieve the mineral composition and content of the core and the three-dimensional distribution of deep minerals.

5.2 Recommendation

As for future development, an integrated management system for the Spectral Crust
project should be established. It will include the following:

(1) Construction of mineral spectral image database

The system will include a mineral spectral image database relevant to the image’s spectral and spatial characteristics. Thus rapid acquisition, reasoning, and discrimination of mineral spectral characteristics will be realized. The database will consist of the following four sub-databases: an integrated pretreatment product database, a hyperspectral standard framing products database, a core catalog database, and a model algorithm database. These will form a basis for automatic extraction and the application of mineral hyperspectral information.

(2) Development of multi-source and multi-scale spectral data processing and analysis subsystem

The multi-source and multi-scale spectral data processing and analysis subsystem will consist of two parts: one for integrated multi-source and multi-scale data and the other for integrated processing and analysis.

Data integration is mainly needed for mineral exploration and multidimensional mapping, and for establishing and exercising uniform standards and regulations of multi-source and multi-scale spectral data. The subsystem aims to fulfill key technologies of fusion and splicing of various sensors and high-resolution spectral images, to realize dynamic integration of satellite, airborne, and ground-based core hyperspectral data, to research dynamic indexing techniques for multi-scale hyperspectral data, core data, and other forms of geological data, to build a data integration model oriented to spectroscopy and mineral identification, and to frame the data storage model. This subsystem will support follow-up spectroscopy, mineral identification, and visual expression of all kinds of heterogeneous data, leading to a logically unified set of standardized data for the study area.

The integrated spectral data processing and analysis consists of six parts. In the first part, a system will be established for satellite, aerial, ground, and core spectrum data, realizing fast spectroscopy and mineral mapping applications after data-centered processing. In the second part, the image data will be preprocessed, including atmospheric, geometric, and spectral correction, and absolute and relative calibration. In the third part, the images will be enhanced and transformed to improve quality and meet the needs of analytical applications. In the fourth part, the classification and identification of mineral resource extraction will be completed according to fine classification criteria and the recognition model for satellite, aerial, ground, and core spectrum data. The fifth part will involve a comprehensive analysis of hydrothermal alteration polymers, detection of mineralization, and identification of spectral information based on a spectroscopy model. Finally, the extracted results will be applied to a geological mapping system after classification and extraction of
information on the rock and mineral distribution, depth, and abundance.

(3) Construction of a crust spectral three-dimensional graphics subsystem

Classification maps will be compiled based on analysis results from multi-source and multi-scale spectral data processing and analysis subsystems. They will then be used as thematic maps of spectral crustal rocks and mineral to extract abnormal pixel spectral curves along with screening and confirmation. The extraction results for a variety of alteration minerals will be obtained after a series of processing steps. Three-dimensional mapping of spectral crustal rock and mineral information will be achieved by analysis of the mapping results combined with integrated satellite, aerial, ground, and core mineral distribution data. A three-dimensional graphics subsystem will be utilized. A mineral three-dimensional distribution model and metallogenic prediction model will be established and combined with the spectral analysis and mapping results. Existing mineral resources, both surface and underground, can be described to 1-km depth, allowing reasonable prediction of the distribution of mineral resources to guide future exploitation.

Research will be based on quadtree and octree data structures and hyperspectral image modeling of the mining area cube and mining cube units. Specifically, modeling will involve three-dimensional interpolation based on drill core real-time measurements of spectral data, spectrum ratio three-dimensional modeling based on drill core real-time measurements of spectral data, and three-dimensional modeling based on geophysical or geological volume data. These modeling procedures will result in three-dimensional maps of hyperspectral data cubes of the earth's crust.

(4) Development of a crust spectral data multidimensional visual expression subsystem

Oriented to spectral crust multidimensional geological information, this subsystem will handle three-dimensional visual integration of the surface and subsurface. It will contain a massive multi-dimensional geological data scheduling mechanism, multi-dimensional geological information composite integrated visualization, a three-dimensional query and display system, and a multi-mode roaming browsing feature. The multi-dimensional geological information visual expression subsystem will consist of five parts: basic calculation modules for grid cell bodies (e.g., grading, gradients, density calculation), mine cube data slice modules (e.g., plans, sections, grid-like maps), a mine cube data slice overlay comparison module, a multidimensional data statistical analysis and data mining module oriented to the mine cube unit, and a mineral interpretation three-dimensional mapping module based on a hyperspectral mineral identification model (e.g., mineral content map, classification map).
(5) Integration of the spectral management system

The integrated satellite, airborne, and ground-based spectral crust management system will be a processing and analysis application platform for the mineral spectral image database, the multi-source and multi-scale spectral data processing and analysis subsystem, the crust spectral three-dimensional graphics subsystem, the crust spectral data multidimensional visual expression subsystem, and the multi-source and multi-scale data. It will have applications in geological prospecting and mineral monitoring.

References


[22] G. Carr, A. Andrew, G. Denton, A. Giblin, M. Korsch, and D. Whitford, "The


[38] S. Fraser, A. Gabell, A. Green, and J. Huntington, "Targeting epithermal
alteration and gossans in weathered and vegetated terrains using aircraft scanners- Successful Australian case histories," 1987.


2-12, 2007.


Résumé, introduction et conclusion en Français

A la fin de ce document, conformément à la règle établie par Aix-Marseille Université, nous avons rédigé en français :
- le résumé
- l’introduction
- la conclusion

de ce mémoire de thèse.
Résumé

Caractérisation des sols par l’analyse d’images hyperspectrales en télédétection

Les images hyperspectrales fournissent des informations intéressantes quant à la composition des sols, en particulier au niveau minéral, ce qui permet de caractériser efficacement les « groupements de minerai » et les « minerais isolés ». Ce travail de recherche avait pour objectif d’établir un système de cartographie 3D des minerais qui intègre des informations de surfaces (acquises par satellite ou à partir d’un aéronef) et des informations souterraines (par forages) à partir de données hyperspectrales. Le travail décrit dans ce mémoire s’articule de la manière suivante :

- Pour la cartographie de surface, nous avons développé et optimisé des algorithmes pour mesurer de manière à la fois précise et homogène au niveau des transitions, le taux de minerais à toutes les longueurs d’ondes (de 0.2 à 12m) à partir de l’imagerie hyperspectrale par satellite et aéroportée. Cela a nécessité de développer des solutions pour décorrélérer les cibles minérales du fond, en ne retenant pas les pixels associés à des taux peu importants de minerai (zones sans végétation). Un travail a été également fait à ce sujet pour améliorer la correction atmosphérique. Nous avons également utilisé le modèle de BRDF de Hapke pour étudier la composition (ou mélange), linéaire et non linéaire, des modèles spectraux, et nous avons développé sur cette base, des algorithmes de séparation des spectres s’appuyant sur des bibliothèques spectrales, ainsi que la profondeur, la position et la forme des caractéristiques d’absorption dans l’infrarouge en « proche du visible » (VNIR), en « ondes courtes » (SWIR) et « thermique » (TIR) pour les minerais.

- Pour la cartographie minéralogique souterraine, nous avons développé un système que nous avons appelé Field Imaging Spectrometer System (FISS) et que nous avons associé au système de forage, dont le verrou scientifique était dans le calcul et la mise en œuvre de la précision sur les produits minéraux recherchés, en particulier pour ce qui est des caractérisations des minerais à partir de l’infra-rouge « ondes courtes » et « thermique ».

- Nous avons mis cela en application par la suite, de manière à mieux comprendre le système minéral, et ce à partir de méthode utilisant les données hyperspectrales. Pour cela, nous avons utilisé les Systèmes d’Information Géographique (SIG), ce qui nous a permis de produire des simulations relatives à l’exploitation minière.
Introduction

Contexte de la cartographie minérale 3D hyperspectrale

La découverte de gisements miniers constitue un élément important de l’essor économique d’un pays, et c’est également un paramètre clé permettant de caractériser les progrès de cette économie. C’est la raison pour laquelle nous nous intéressons au problème de la cartographie des gisements miniers.

La plupart des lieux où il y a matière à prospec ter sont éloignés et difficilement accessibles. Et les résultats de la prospection (carottage, puits de mines) ne sont pas toujours probants. Depuis quelques années, la télédétection est devenue le mode opératoire privilégié pour extraire l’information relative à la cartographie minière et, pour être plus précis, la télédétection à base d’imagerie hyperspectrale est devenue l’outil principal d’analyse des ressources terrestres (cartographie minière mais également géologie et exploitation des terres).

Les minerais sont présents dans toutes les roches et dans tous les sols ; ils sont donc à l’articulation de l’exploration minière et du développement durable. Une cartographie minière 3D précise permet également de mieux comprendre les processus d’échanges au niveau minéral, et des systèmes géologiques en général, en particulier pour promouvoir une exploration durable liée à la reconnaissance des processus de minéralisation (ou de dépôts de minerais).

Le Centre d’Excellence pour la cartographie minérale 3D (C3DMM : [http://c3dmm.csiro.au](http://c3dmm.csiro.au)) affirme que, dans le futur, l’industrie minière s’appuiera systématiquement sur cette cartographie, en utilisant des cartes 3D obtenues à partir d’imagerie hyperspectrale pour prospecter de manière spécifique, et ce avec un coût financier et environnemental réduit. Les travaux du C3DMM sont axés sur une « Vision 2020 » avec la création d’un site Web qui sera public, accessible, dont les informations seront traçables et mesurables, pour produire une carte minérale 3D de l’Australie obtenue à partir des carottages, mais aussi et surtout des données acquises « de manière adaptée aux géosciences » obtenues par télédétection aéroportée ou satellitaire. En Chine, un projet analogue, intitulé « Spectral Crust » est en place et s’appuie essentiellement sur l’imagerie hyperspectrale. Ce projet s’est fixé cinq buts majeurs, qui sont de trouver des solutions aux problèmes suivants :

- Minéralogie sous-terrain e : il s’agit de déterminer la signature hyperspectrale associée aux carottages et de produire ainsi une carte « continue » (i.e. sans « couture »).
- Minéralogie de surface : il s’agit de produire une carte minérale de surface à partir de données de télédétection (aéroportée et satellitaire).
- Systèmes d’Information : il s’agit de développer des algorithmes permettant d’obtenir des mesures précises sur l’information minérale, d’établir des interfaces entre les différents formats de données, et de véhiculer l’information pertinente dans les systèmes d’accès à ces données (sur le Web).
- Cartographie minérale 3D : il s’agit de développer des modèles 3D liés à la minéralogie.
- Systèmes minéraux : il s’agit d’améliorer la connaissance sur la formation des dépôts minéraux et leurs possibilités d’exploitation.

Cette thèse a pour objectif de montrer comment on peut extraire l’information des images hyperspectrales et comment on peut la corréler aux prélèvements sur le terrain.

**Pertinence de cette voie de recherche**

La spectroscopie sous forme d’images peut être utilisée pour caractériser la minéralogie surfacique à travers les caractéristiques spectrales de l’absorption des matériaux observés. Suivant la nature de la surface, des processus électroniques et vibratoires produisent une absorption dans différentes fréquences, permettant ainsi l’identification de matériaux organiques et non organiques. Ces caractéristiques d’absorption se situent principalement dans le domaine du visible et du proche infra-rouge. Cette caractérisation sera complexe lorsque les minéraux seront mélangés, ce qui est en général le cas dans la nature : ils pourront être intimement mélangés mais aussi, dans certains cas, l’un d’eux pourra recouvrir l’autre, par exemple ; la granularité (« taille des grains ») affectera également la réponse spectrale et sera à prendre en compte ; enfin, cette réponse dépendra non seulement de la composition chimique mais aussi de la structure du matériau. Malgré ces difficultés, il est possible d’extraire une information spectrale au niveau moléculaire qui produise un outil efficace pour la cartographie minéralogique.

La spectroscopie sous forme d’images fournit une base intéressante pour analyser et cartographier les associations de minéraux. La description des caractéristiques d’absorption (profondeur, largeur, asymétrie) permet de caractériser le spectre en accord avec celui des matériaux de base, simples et connus.

La télédétection pour la géologie est un « problème mal posé » dans la littérature. Tel qu’il est donné, ce nom suppose que les données de télédétection (terrestres, aéroportées ou satellitaires) sont utilisées pour étudier la géologie. Traditionnellement, la géologie s’intéresse à la composition, à la structure et à l’histoire de la terre. Toutefois, de nos jours, la géologie s’intéresse de plus en plus
aux processus qui ont permis de former la terre et les autres planètes, ce qui permet de dire que la géologie est de plus en plus multidisciplinaire et positionnée sur des problèmes sociétaux. La plupart des travaux de télédétection pour la géologie dans le proche infra-rouge (VNIR), dans l’infra-rouge ondes courtes (SWIR), dans l’infra-rouge moyen (MIR) et dans l’infra-rouge thermique (TIR) ont été menés par les pionniers du domaine que sont Hunt et Salisbury, qui ont méticuleusement mesuré la réponse spectrale des roches et des minéraux à partir de systèmes d’acquisition aéroportés et satellitaires. Les géologues utilisant la télédétection ont activement contribué au développement des capteurs actifs (radar à synthèse d’ouverture SAR et inSAR) et des capteurs passifs (multispectraux et hyperspectraux dans les parties du spectre allant du proche infra-rouge à l’infra-rouge thermique).

**Etat de la recherche dans le domaine**

**La télédétection hyperspectrale en géologie**

Pendant de nombreuses années, les images de télédétection ont été soit monochromatiques soit multispectrales (i.e. à une fréquence donnée, ou sur un ensemble de bandes spectrales discrètes et en petit nombre). Les données et images produites par les systèmes d’imagerie multispectrale (aéroportés ou satellitaires) ont été du type « 4 bandes MSS » (multispectral scanner) et « 7 bandes TM » (Thematic Mapper) « Landsat data », ou du type « 3 bandes SPOT images », et ont constitué l’essentiel des données de télédétection pendant des décennies. Typiquement, la largeur de bande de ces capteurs est assez large (supérieure à 0.07 µm). À l’opposé, les données hyperspectrales sont acquises à une plus grande résolution spectrale (largeur de bande plus étroite, typiquement 0.02 µm ou moins) et ces bandes sont contiguës.

Le premier spectromètre d’imagerie embarqué a été l’imageur hyperspectral LEWIS (HSI) de la compagnie TWR ; il a été lancé en 1997 mais a été défaillant. Dans le cadre du programme du nouveau millénaire (NMP), la NASA a lancé Hyperion avec Earth Observing EO-1. Hyperion (Pearlman et al., 2003), s’appuyant sur les concepts de LEWIS, a 220 bandes spectrales (de 0.4 à 2.5 µm), une résolution spatiale de 30m et des images de 7.5km par 100km. Quant à l’Agence Spatiale Européenne (l’ESA), elle utilise le CHRIS (Compact High Resolution Imaging Spectrometer), sur le Proba-1, qui mesure la réflectance spectrale directionnelle à partir de vues multiples et des différentes géométries d’illumination (de 0.415 à 1.050 µm) sur 19 bandes, avec une résolution spatiale de 20m au nadir, et une fauchée de 14km.

ASTER (Advanced Space borne Thermal Emission and Reflection Radiometer) a été lancé en 1999. ASTER travaille en multispectral en couvrant des zones de 60km par 60km mais il dispose de 14 bandes qui couvrent la totalité de l’infra-rouge (du VNIR au TIR). Les trois bandes du VNIR ont une résolution spatiale de 15m, les six bandes
du SWIR en ont une de 30m et les cinq bandes du TIR ont une résolution de 90m.

L’imagerie hyperspectrale satellitaire est devenue une réalité en novembre 2000 avec le lancement réussi de Hyperion sur EO-1, et le fait qu’il ait été effectivement opérationnel dès son lancement.

Mentionnons enfin SEBASS qui est un capteur hyperspectral avec 128 bandes et une résolution spatiale beaucoup plus fine (de 2 à 5m).

**La télédétection aéroportée en géologie**


Le système AVIRIS, qui a été opérationnel en 1987, a été l’un des tout premiers systèmes d’imagerie hyperspectrale embarqué à être utilisé pour des applications dans le domaine de la géologie. Grace à la structure de bandes contiguës du système AVIRIS, il est possible de résoudre des problèmes difficiles, et « subtils », de caractérisation d’absorption des différents minéraux. AVIRIS a 224 bandes contiguës, de 0.60 à 2.5 µm, avec une résolution spectrale de 10nm, et une résolution spatiale de 4 à 20m, suivant l’altitude de vol de l’aéronef.

A l’heure actuelle, il existe une grande variété de systèmes d’imagerie spectrale (dans le VNIR et le SWIR) qui sont aéroportés. En particulier, ProSpecTIR-VS, de la
société SpecTIR, LLC (www.spectir.com), est un système personnalisé qui intègre différents système AISA de SPECIM (Eagle et Hawk) pour produire des capteurs haute performance qui permettent l’acquisition simultanée dans une bande spectrale allant de 0.4 à 2.45 µm : les deux spectromètres imageurs sont « alignés » pour produire un cube de données des 320 pixels de côté ; à cela, il faut ajouter qu’une instrumentation performante permet (selon l’altitude de l’aéronef) d’obtenir une résolution allant de 0.5 à 5 m.

Hymap est un capteur (imageur) hyperspectral aéroporté, avec 126 bandes, couvrant un spectre allant de 0.45 à 2.5 µm, avec des largeurs de bandes de 15 à 20 nm, et une résolution spatiale de 3 à 5 m. Hymap a un excellent rapport signal sur bruit (500 :1) ce qui en fait un outil très puissant pour une analyse fine de la minéralogie de surface.

**Analyse spectrale des « champs de minéraux »**

Avec l’arrivée de spectromètres et de spectroradiomètres très compacts et sophistiqués, l’utilisation de la spectroscopie est devenue une technique robuste pour la prospection minière et la cartographie minéralogique. C’est également un outil très puissant pour étudier les interactions « matière – énergie » sur des échelles allant de quelques centimètres à plusieurs mètres. Toutefois, il est indispensable, pour exploiter cette technologie dans ce domaine, d’en maîtriser parfaitement chacun des maillons qui sont la géométrie des capteurs, la granularité, le calibrage de l’instrument, la procédure d’acquisition spectrale, ainsi que les algorithmes de séparation de sources, etc.

De tels systèmes d’imagerie spectroscopique au sol existent, mais ils ont vite montré leurs limites et ouvert le champs aux systèmes embarqués (aéroportés et satellitaires). Ces limites sont le fait du coût et de la faible couverture de ces systèmes au sol, qui conservent toutefois un intérêt, par exemple pour établir la validation d’une acquisition aéroportée ou satellitaire (i.e. il s’agit d’une forme de « vérité terrain ») ou pour avoir, dans certains cas, une très haute résolution spatiale qu’on ne pourrait avoir autrement.

Des mesures terrain ont été effectuées en utilisant un spectromètre portable, le FieldSpec 3 Analytical Spectral Device (ASD). Le spectre échantillon a été à la fois examiné et étudié, manuellement et à travers un algorithme dédié faisant partie du logiciel ENVI de manière à définir au mieux les « classes de spectre » présents dans l’échantillon. Cela permet de produire un « cube image » de mesures spectrales qui permettra ensuite une analyse plus pertinente avec un capteur aéroporté ou satellitaire. Finalement, ce « cube image » permettra de représenter le spectre de manière totalement « ponctuelle » sans être perturbé par les interactions avec les voisins (comme c’est le cas pour l’imagerie hyperspectrale embarquée). Le spectre est ensuite analysé et « classifié » avec un algorithme SFF (Spectral Feature Fitting).
Analyse spectrale des carottages et des affleurements

La spectroscopie a également été utilisée pour l’analyse des carottages et des affleurements. Les travaux de recherche décrits dans ce manuscrit montrent l’intérêt d’intégrer les différentes modalités (aérienne et satellitaire, par carottage, par étude de surface sur le terrain).

Ainsi, par exemple, le capteur ProSpecTIR-VS a opéré en trois modes : aéroporté (résolution de 1 m), pour l’analyse de carottages (résolution de 2 mm) et pour l’inspection des murs de la mine (résolution de 4 cm). D’autres expérimentations de ce type ont été faites, également, avec des instruments de natures différentes, permettant de compléter l’information acquise par l’un d’eux.

Cartographie minérale 3D

La raréfaction des ressources minières a amené Graham Carr (Australie) à définir le concept de « terre de verre » qui consiste à enlever une « première couche » d’un kilomètre pour cartographier les ressources (« méga-dépôts ») se trouvant à ce niveau-là. D’autres programmes de ce type existent, tels le « Mineral Down Under » (toujours en Australie) qui s’articule autour de trois sous-programmes : ROES (une méthode d’exploitation minière à bas coût et contrôlée à distance), analyse hyperspectrale et interopérabilité au niveau des données géoscientifiques.

En Chine, le projet « Chang’e Moon » a mis en place l’utilisation de technologies spatiales dans ce domaine (satellites, capteurs, lancement et contrôle de la navigation de fusées). Et l’un des aspects sur lequel l’accent a été mis est celui de l’imagerie hyperspectrale.

Structure du manuscrit

Le manuscrit est structuré en cinq chapitres. Après un premier chapitre d’introduction, nous présentons (dans le deuxième chapitre) la théorie de la cartographie minérale et les bases du traitement des données hyperspectrales. Le troisième chapitre est dédié à la cartographie surfacique des données hyperspectrales, à travers le traitement des données satellitaires, aéroportées et acquises sur le terrain. Dans le quatrième chapitre, nous traitons de la cartographie à partir des carottages et en utilisant un spectromètre spécialement conçu à cet effet. Le cinquième chapitre présente les conclusions de ce travail et les axes de recherche qui devraient être développés par la suite.
Conclusion et Axes de Recherche

Conclusion

Tel que cela a été défini dans sa stratégie au niveau national, la Chine souhaite renforcer les aspects technologiques et applicatifs innovants dans le domaine de la détection des ressources minières. Pour cela, l’accent a été mis sur quelques secteurs clés tels que le développement de l’imagerie hyperspectrale satellitaire et aéroportée, les plateformes au sol et les carottages pour valider les modèles sur les données acquises en « spatial » (vérité terrain), et tout l’aspect compilation, analyse, intégration des données acquises.

Dans ce manuscrit, nous avons présenté comment nous pouvons utiliser toutes les modalités d’acquisition de données, et en particulier les données image hyperspectrales, et établir à partir de cela une base de données spectrale. Dans un futur proche, nous développerons les éléments technologiques pour disposer d’une plate-forme permettant le contrôle des ressources minières et énergétiques, de manière à ce que les utilisateurs puissent y accéder de manière efficace, avec un modèle économique permettant de pratiquer une exploration minière et de sources d’énergie, en s’appuyant sur des moyens « raisonnables » et contrôlés.

Dans ce manuscrit, nous avons tout d’abord fait un « état des lieux », en analysant les travaux de recherche dans le domaine, que ce soit au niveau technologique ou au niveau des méthodes utilisées. Puis, nous avons montré comment on pouvait mettre en place un premier système de gestion des données, avec en particulier les images hyperspectrales aéroportées et satellitaires. Nous avons également développé une instrumentation au sol pour valider les modèles à travers la vérité terrain. Et nous avons enfin mis en place un système pour l’analyse et la représentation 3D d’une cartographie des minéraux en profondeur.

Axes de recherche

La poursuite de ce travail, que ce soit en matière de recherche ou en termes de développement, a déjà fait l’objet d’une réflexion, puisqu’il s’inscrit dans le projet « Spectral Crust ». Nous proposons donc cinq axes de rechercher et de développement.

1. La construction d’une base de données image pour la caractérisation spectrale des minéraux
2. Le développement de sous-systèmes de traitement et d’analyse des données
images multi-sources et multi-échelles
3. La construction d’un système de représentation 3D spectral de la croûte terrestre
4. Le développement d’un sous-système permettant de visualiser les paramètres multidimensionnels de la croûte terrestre
5. L’intégration dans un système de gestion spectrale.

Reprenons à présent et détaillons chacun de ces points.

La base de données images s’articulera autour de quatre « sous bases de données » dédiés respectivement aux données issues du prétraitement, aux images hyperspectrales elles-mêmes, au catalogue noyau, et aux algorithmes et modèles.


La construction du système de représentation graphique 3D spectral de la croûte terrestre aura à effectuer de la prédiction et de l’interpolation (à partir des carottages et autres données ponctuelle) en s’appuyant (suivant l’épaisseur de la couche) sur une structure de quadtree ou d’octree. L’objectif sera d’obtenir des « cartes » 3D sous forme de cubes de données hyperspectrales.

La visualisation des données multidimensionnelles n’est pas une tâche évidente car il s’agira de permettre une interprétation et une identification des données et de l’information extraite de ces données.

Le dernier point (intégration dans un système de gestion spectrale) n’est pas à proprement parler un axe de recherche, mais il est important de le mentionner car il s’agit d’une tâche de développement importante pour le futur du projet « Spectral Crust ».