



# Spectral Analysis and Unmixing of Iron Ore Based on MATLAB and ENVI

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## ABSTRACT

With the development of industrial technology, qualitative and quantitative analysis of iron ore has become more and more important. Qualitative analysis mainly includes artificial empirical models for the identification of iron ore to matching algorithm models, to quantitative analysis from traditional chemical method analysis to today's hyperspectral remote sensing analysis. The main contents of the thesis include:

1. The first part is about the algorithm implementation of MATLAB for spectral analysis and spectral unmixing. The software module design includes spectral data preprocessing module, iron ore type analysis module and iron ore total iron content quantitative analysis module. Each module is an integral part of the overall software module system.

2. The second part contains the pre-study and data processing method design for iron ore species identification module. Firstly, the spectral curves of the most representative iron ore are displayed, and the spectral characteristics of each iron ore are clearly understood. The regularity and difference of these spectral features are summarized, and a spectrum containing the current common iron ore is established. The library then is used for matching recognition algorithm to process and analyze the spectrum of the iron ore, and obtain the matching result, thereby realizing the end iron ore type analysis module.

3. The third part is to focus on the analysis of total iron content of magnetite in the analysis module of iron ore total iron content and propose the method of inversion of magnetite content at the current stage, focusing on the use of magnetite samples for spectral unmixing. Their total iron content is then extracted, and the nonlinear results are compared with traditional chemical methods. The accuracy verification analysis is performed by XRF method.

**Keywords:** Iron ore; Hyperspectral remote sensing; Quantitative analysis; Qualitative analysis; Total iron content; Spectral unmixing

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# 1 Introduction

## 1.1 Research background

The generation of the spectrum cannot leave the light. In an experiment in 1666, Newton discovered that sunlight can be broken down into seven colors of light by prisms, and the spectrum is composed of these colorfully decomposed lights. Modern spectroscopy is created by this great experiment. Spectroscopy mainly studies the principle of each material spectrum and the interaction between spectra, and spectroscopy also provides a new qualitative analysis and quantitative analysis method for iron ore analysis<sup>[1]</sup>.

### 1.1.1 Spectral characteristics of minerals

The core of this paper is to study the spectral characteristics of iron ore. But because the difference in spectrum between different types of substances is much higher than the spectral difference between substances in the big categories. For example, the spectral characteristics of plants and minerals are significantly distinct, but the spectral characteristics of oak and pine leaves are obviously similar, with only minor differences.

Studies have shown that the spectral characteristics of minerals in the range of  $0.4\mu\text{m}$ - $1.3\mu\text{m}$  are mainly affected by iron and some transitional metal elements in minerals. These elements exist in the lattice structure of minerals in the range of  $1.3\mu\text{m}$ - $2.5\mu\text{m}$ . The spectral characteristics in the interior are determined by the  $\text{CO}_3^{2-}$ ,  $\text{OH}^-$  and the  $\text{H}_2\text{O}$  molecules that are not necessarily present in the mineral composition. The spectral characteristics in the mid-infrared and far-infrared bands of  $3\mu\text{m}$ - $5\mu\text{m}$  are from Si-O, Al-O, etc. The vibration mode of the molecular bond is determined. Therefore, the influence factors of minerals in each band range are different<sup>[2]</sup>.

The mechanisms that determine the spectral characteristics of minerals are electronic transitions and lattice vibrations. Mineral spectroscopy has mechanisms that

determine the spectral characteristics of minerals and factors that influence the spectral characteristics of minerals. The spectrum of each substance is related to their physical properties. For most non-mineral molecules, energy is composed of electron energy, vibrational energy, and rotational energy. But the mineral molecules do not contain rotational energy. The energy difference between the vibrational levels is called  $\Delta E$ , which is typically between 0.25 and 1.00 eV, depending on the calculation. The spectrum of the corresponding energy's difference is mostly in the range of the near-infrared and mid-infrared bands. The energy difference between the electron levels is larger than the energy level of the vibration level, and the corresponding spectrum is located in the near-infrared and visible-light range<sup>[2]</sup>.

Electronic transitions are due to the transition of energy between energy levels and energy levels, through their absorption and radiation at specific wavelengths, resulting in corresponding spectral characteristics. For example,  $\text{Fe}^{2+}$ , when it is arranged in a regular octahedron, produces a broad strong band around 1.0 $\mu\text{m}$ . When its arrangement shape is a distorted octahedron, two energy level transitions are generated, and one will produce strong absorption near 1.0 $\mu\text{m}$ , and another one will produce weak absorption near 1.8 $\mu\text{m}$ .  $\text{Fe}^{3+}$  has symmetry, so the electronic transition produced by it is a transitional form of confinement, and its spectral characteristics are weak band and dispersed absorption band, which causes the spectral sharp drop in the visible spectrum of its mineral spectrum. The appearance of the absorption peak is about 0.5 $\mu\text{m}$  and near 0.9 $\mu\text{m}$ <sup>[2]</sup>. Due to the different structures of various crystals, the fundamental frequency positions generated by lattice vibration are also different. An integer multiple of the fundamental frequency is an excitation of the received external energy. When this occurs, a combined spectral band is generated, the position of which is at or near the fundamental and multiplier positions. The spectral characteristics produced by lattice vibration are related to its unique lattice structure, so the structure is closely related to the properties exhibited by the object. It is concluded that there are four main elements

in the crystal lattice, namely  $\text{CO}_3^{2-}$ ,  $\text{OH}^-$ ,  $\text{H}_2\text{O}$ ,  $\text{Si-O}$  and their fundamental frequency ranges are also different<sup>[2]</sup>.

Factors that affect the spectral characteristics of minerals include weathering, surface structure, surface color, and atmospheric environment. Weathering has a great impact on mineral changes and even changes mineral traits. Hydrates produced by the weathering of minerals can erode the rock surface or the soil surface. Through the action of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$ , the spectral curve changes greatly in the visible range, while it changes little in other parts. For transparent materials, it is typical to reduce the particle size, increase the reflectivity, and reduce the spectral characteristic contrast. The mineral surface structure has a certain influence on the spectral reflectance of minerals. When the mineral composition is basically the same, the particle size reduction of the mineral particles will lead to an increase in the spectral reflection intensity, because the smaller the particle size, the stronger the scattering of incident light and reduced matting. In the case of oblique incidence, the shadow area of fine minerals or powdered minerals becomes smaller, thereby enhancing the reflection intensity of the mineral surface. Then, the color of minerals is a concentrated expression of mineral content, metal impurities and organic matter content. Different kinds of minerals are different in color. Dark minerals contain a high level of organic impurities and very low mineral reflectivity, which also makes it difficult to analyze dark minerals. Light minerals contain less organic matter and have higher reflectivity. Impurity components in minerals are often reflected in the color of the minerals, which in turn affects the spectral reflectance of the minerals, sometimes even offsetting the spectral characteristics of the mineral itself. Therefore, the study of dark minerals requires the development of new methods to eliminate the effects of organic matter. Finally, measured under natural light, the spectrum of minerals is significantly affected by environmental conditions, such as the limits of the atmospheric window, random changes in wind, temperature, pressure, and visibility. The most obvious one is the atmospheric influence, because the atmosphere

can change the spectral distribution of solar radiation, so that the direct radiation energy decays and the scattered radiation increases<sup>[2]</sup>.

#### 1.1.2 Introduction of iron ore

The most important raw material for the iron and steel industry and the most important core ore resource for national economic development is iron ore. Iron ore contains iron and non-ferrous minerals, and is also a general term for iron-containing minerals. Iron ore is not demanding on economic conditions, and can be developed and utilized at any time. It has a wide range of commercial and industrial values, and there are many industrial processes related to iron ore. In terms of geology, the geological change of iron ore is time consuming. During this period, it is mixed with other minerals and elements mechanically or chemically. The resources of places where iron ore is concentrated are often exploited by the industry, and the natural minerals are not able to be exploited if the distribution is relatively evacuated.

There are more than 300 kinds of iron ore currently discovered in the Earth's ecological circle, and the most representative of which are magnetite, hematite, limonite, siderite, goethite, etc. In certain cases, they can be exploited by industrial production. In this particular case, they become iron ore, such as the most typical magnetite and hematite. China also has many iron ore resources, and it has its own characteristics. In China, the percentage of total minerals in the poor ore is 80%. The upper half of these poor ore deposits are mainly hematite, and the lower half is mainly magnetite. Moreover, the types and quantities of ore that are multi-element symbiosis in China are numerous, and the ore bodies are complex compared with some countries with scarce resources. China has the unique advantage in industrial production. The main producing areas of iron ore in China are in the Inner Mongolia region and the northeast region. Therefore, the use of iron ore as the research object is significant and the research results may contribute to actual industrial production.



The overall spectral characteristics of iron ore are mainly determined by  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$  in iron ore. It is found that the absorption peaks of  $\text{Fe}^{2+}$  are 430nm, 450nm, 550nm, 1000nm~1100nm, and the absorption peaks of  $\text{Fe}^{3+}$  are 400nm, 450nm, 700nm and 870 nm. Two kinds of iron ions have a certain influence on the spectral characteristics of iron ore. Different iron ores also have different associated mineral combinations, and associated minerals refer to the general term for deposits containing other minerals. Mines generally contain a large number of associated minerals, but the content of associated ores is generally not high relative to important minerals. Mining separation is generally achieved with high utilization value. China has many high values associated mineral resources, such as the Baiyune mining area in China. If the associated minerals are present in a deposit with a high mineral content, the associated mining value is not high. But when it exists in other mines with little content in the main mining, the value of associated minerals can be reflected.

### 1.1.3 Analysis of iron ore

For the analysis of iron ore, it is mainly the analysis of its total iron content. Analysis of iron ore now is mainly chemical methods and instrumental analysis methods, and the instrument method contains a variety of instruments, such as hyperspectral spectrometer or XRF handheld detection device. At present, the most frequently used method for inversion of total iron content by chemical method is potassium dichromate titration. The core method is to mix and dissolve sulfur-phosphorus mixed acid and sodium fluoride, and react with tin oxide to reduce the selectivity with  $\text{Fe}^{3+}$ . The remaining  $\text{Fe}^{3+}$  was reduced with titanium trichloride and sodium tungstate was used as an indicator. Excessive  $\text{Ti}^{3+}$  reduction of sodium tungstate produces "tungsten blue", and finally the sample is titrated with potassium dichromate to a stable purplish red. Its formula is as follows:

$$\omega(\text{Fe}) / \% = \frac{c \times (V - V_1) \times 55.85}{m \times 1000} \times 100$$

C ——— Concentration of potassium dichromate standard solution. mol/L

$V$  —— Volume of the potassium dichromate standard solution consumed when titrating the sample. ml

$Vl$  —— Volume of potassium dichromate standard solution consumed when titrating a blank solution. ml

$m$  —— weigh the mass of the sample. g

55.85 ——Molar mass of Fe.mg/mol

Compared with the traditional potassium dichromate titration method, the instrument analysis method can identify the sample faster, the processing is relatively simple, no complicated process is required, and the accidental error is small. This design focuses on hyperspectral instrumental analysis. Hyperspectral remote sensing, as its name suggests, is a technique that uses a very narrow and continuous spectral channel to continuously image an object. From the visible light band to the short-wave infrared range, it has micron or even Nano-scale spectral resolution. It has many characteristics of identifying bands, and the number of spectral channels is more than hundreds, and the spectrum is often continuous. Therefore, the core of imaging spectral remote sensing is hyperspectral remote sensing technology. In China and abroad, hyperspectral technology is developing rapidly and has received a lot of attention from industry. It integrates many modern technologies, such as computer programming technology, micro-sensor detection technology, precision optical instrument technology, digital signal processing and detection technology. The principle of imaging is to use nanometer-scale spectral resolution. In the imaging process, it uses imaging spectrometer to image the ground object simultaneously with tens or hundreds of bands at nanometer spectral resolution, and can obtain continuous spectrum of ground objects. The information contains the synchronous acquisition of ground space information, radiation information and spectral information, and thus has great application value and broad development prospect in the field of iron ore identification analysis.

At present, there are many kinds of iron ore spectral analysis techniques, and most of them are still developing steadily. They all continue to improve with the advancement of space technology, analytical methods and technologies. Because a large number of applications in the field of iron ore analysis require the application of mathematical

statistical analysis methods, computer programming methods and spatial visualization methods, the application of these methods is closely combined, and they have made great contributions to hyperspectral application technology. Among them, the following technologies are commonly used in iron ore analysis.

The core of the spectral unmixing technique is to analyze the mixed pixels to determine the percentage of mixed pixels in the number of endmembers. Through this technology, the reflectance spectrum of a remote sensing image or mixed sample can be analyzed and identified, and the content of each endmember can be quantitatively analyzed. This is also the core technology of the project. The imaging unit of a hyperspectral imager is called a pixel, and one or more features can be recorded in each pixel<sup>[1]</sup>. A pixel that only records a feature is called a pure pixel. Conversely, if the spectrum of a pixel species contains spectra of multiple species, such a pixel is called a mixed pixel. The study of hyperspectral technology cannot avoid solving the problem of mixed pixels. There are three main reasons for the formation of mixed pixels. The first is the mixed effect of the hyperspectral sensor, and the second is the mixing effect in the atmospheric transmission process, and the third is due to the limitation of the spatial resolution of the current sensor, which is insufficient to guarantee each pixel is pure pixel<sup>[1]</sup>. However, since the recognition of image at the pixel level is very difficult, the spectral unmixing technique is created to solve this problem. This technique decomposes mixed pixels into endmembers and abundances. Different features have different spectral characteristics, and each feature is called an endmember, that is, different features represent different endmembers. The abundance represents the mixing ratio corresponding to the spectrum of each feature. Therefore, spectral unmixing technology has an unshakable position in the study of hyperspectral images<sup>[1]</sup>.

There are also some methods that are equally important in spectroscopy. Firstly, the spectral differentiation technique calculates the differential value of the reflection spectrum by different order, and uses mathematical simulation to determine at which point the spectrum is bent, the extreme points of the reflectivity, and the specific position of these points. This technique is susceptible to change in the curve and the mean of compression. Spectral differentiation techniques can generally be used to

eliminate linear or near-linear conditions and to remove the effects of noise on the acquired spectrum. However, the method must be used to obtain the non-linear spectrum. Then, Spectral matching technology mainly matches the acquired sample spectrum with the reference spectrum, or matches and identifies with a spectral library to determine their similarities and differences. Using this technique, the empirical model can be eliminated to judge the type of sample and improve the speed and accuracy of sample recognition. Spectral matching technology has a very important position in the field of geological mineral identification, especially the identification of iron ore. Spectral feature extraction, as its name suggests, is a feature of extracting features from the spectrum. The attributes and characteristics of an object are called features. One type of feature extraction is to extract a spatial sample from the area to be analyzed according to the extraction rule. This process can also be called band acquisition. Another category is to find a correlation from an original area to be analyzed and a new area to be analyzed, and to perform band acquisition in the new analysis area.

## 1.2 Research status at home and abroad

At present, research on spectral unmixing at home and abroad is maturing. Representative research institutions in China include Wuhan University, the Institute of Remote Sensing of the Chinese Academy of Sciences, the Institute of Electronics of the Chinese Academy of Sciences, and the China University of Mining and Technology. Representative research institutions abroad include the University of Maryland, the University of Lisbon, and the University of Strathclyde<sup>[1]</sup>.

### 1.2.1 Research status of spectral unmixing

Spectral unmixing includes endmember extraction and abundance inversion. They are all indispensable parts of spectral unmixing. Endmember extraction is generally based on two models, statistical and geometric<sup>[1]</sup>. The abundance inversion generally uses the least squares method, and the least squares method is also divided into different least squares methods according to different constraints<sup>[1]</sup>.

In spectral unmixing, the quality requirements for endmember extraction are very high. The quality criteria for selecting endmembers include the number of endmembers and the spectrum of the endmembers. Logically speaking, if the number of endmembers is less than or equal to the number of bands plus one, spectral unmixing can be performed. However, due to the interference factor between the end bands, the selected endmembers should not be too many, otherwise the error will be very large.

The determination of the endmember type should be the effective component of the representation of most of the cells in the corresponding region of the image. The determination of the number of endmembers should be consistent with the authenticity of most pixels in the region. Too small number of endmembers belonging to other types will be included in the endmember type to be decomposed, resulting in a large component RMS. However, too many quantities can make the model sensitive to equipment noise, air pollution, and the spectrum itself, resulting in component errors. Through the extraction of the endmembers, the pure pixel spectrum of magnetite can be extracted from an actual iron ore sample, and then the abundance of magnetite can be calculated by abundance inversion to calculate the magnetite ore sample. The ratio of the whole iron can be obtained.

The hybrid model is divided into a linear model and a nonlinear model. They are the two most commonly used models for hyperspectral image mixing pixel decomposition. Both models include endmember extraction, which extracts the spectrum of pure features, and solves the abundance of each endmember. Decomposition models mainly include linear mixed spectral models, fuzzy supervised classification models, and neural network models. Among them, the linear model is more commonly used. The linear model assumes that different substances do not interfere with each other and have no interaction. The spectra of pixels in the same region are linear combination models of pure mineral spectra, which can be weighted according to their composition ratio. Mixed pixel decomposition is generally based on image preprocessing such as: radiation correction, geometric correction, atmospheric correction and so on. The process is to first obtain the end-spectrum from band library

or experimental data, and then select a decomposition model to perform mixed pixel decomposition.

### 1.2.2 Research status of Iron ore core catalog

Iron ore core cataloging is an important method for spectral information extraction. The reserves of mineral resources in China are very large. At present, the catalogue and analysis of iron ore spectra are still based on traditional methods. The research on surface minerals and rocks is very scarce. The hyperspectral core cataloging technology is still immature, and the relevant literature is also very few. In the geological survey, the most important part is the acquisition of the core. The core is a very valuable and important research sample, and the acquisition of the core requires the support of drilling technology, but drilling is a costly technology, so this has caused a bottleneck in the implementation of technology. Core cataloging often uses manual cataloging methods when the technology is still immature, but the artificial method has very high time cost and labor cost, labor instability, and it also costs a lot of money for iron ore analysis, and the core data cannot be wholly obtained<sup>[21]</sup>.

Many countries in the world have developed new technologies that have their unique advantages. Kruse from the University of Colorado designed a PIMA hyperspectral mineral mapping technique for core cataloging. The advantages of this technology are low cost, automated operation, long-term maintenance, high production efficiency, and the identification of core mineral types is non-destructive, and it can visualize the obtained two-dimensional data, quantitative and semi-quantitative analysis of mineral content, and it can also identify minerals that are difficult to identify by traditional methods, such as dark minerals. The Australian Science and Technology Organization has released the CSIRO Hyperspectral Core Recording System, which is currently being promoted on a large scale. The UK and Germany also have their respective technical systems, namely Spectra-Map Hyperspectral Core Recording System and Multi-Sensor Core Logger Hyperspectral Core Recording System.

### 1.2.3 Research status of surrounding rock alteration

Surrounding rock alteration is also an important phenomenon for studying iron ore. Surrounding rock alteration has been an important method for mineral exploration in the past 100 years. The metal and non-metallic deposits discovered by this method are very numerous. For example, Mexico's large platinum mine, China's Tongguanshan copper mine, Russia's most porphyry copper mine, Utah's large aluminum mine, Western Australia's giant gold mine, Mexico's large platinum mine, the United States' many white tungsten Mines, corundum mines in Kazakhstan, and most of the world's tin mines, are large mining areas detected by wall rock alterations. Mineral alteration information is an important information basis for prospecting, but these factors are often interfered by other factors, such as other feature information, spatial resolution of remote sensing, spectral resolution and so on. Scientists in various countries are studying new technologies to improve or eliminate the effects of these interfering factors.

### 1.3 Problems at the current stage

There are various problems regarding the extraction of information from iron ore. For example, the spectral information extraction of the representative dark minerals in iron ore is still difficult, and it is difficult to extract effective spectral features. This is because the spectral reflectance of dark minerals is very low, and it is almost impossible to obtain the reflection spectrum of the target. It is possible to determine the content of each element by chemical methods, and to design a new method for its spectrum acquisition. And the iron ore spectral analysis is still based on matching identification, and there are few quantitative analysis studies. At present, there is no software and hardware technology for the actual mine production.

### 1.4 Chapter arrangement

The sections of this report are organized as follows. The first chapter is mainly to introduce the research background and the research status at home and abroad as well as the problems existing at the current stage, which are the mainly mineral spectral characteristics, introduction of iron ore and its analysis methods, endmember extraction

abundance inversion and several methods for identifying iron ore. The second chapter is the realization of the algorithm of iron ore analysis and unmixing in MATLAB. The third chapter is to establish a library of iron ore spectra and analyze their spectral properties. The fourth chapter combines experimental data samples and laboratory analysis results to deeply analyze the spectral characteristics of magnetite, invert the total iron content, and verify the accuracy. The fifth chapter is the conclusion and outlook.



## 2 Analysis and inversion of iron ore based on MATLAB

Through the module implementation of MATLAB software, a relatively complete iron ore analysis and inversion system can be constructed to achieve one-click processing on the computer side. The software processing module includes a spectral data preprocessing module, an iron ore analysis module, and a full iron content inversion module.

### 2.1 Spectral data preprocessing module

This module is the basis for the analysis of iron ore samples. By preprocessing the spectral data, we can initially analyze the wavelength range, center wavelength, peak reflectance and so on of iron ore. In this module, there are several functions that can be implemented, including reading the spectral library, displaying the spectrum, exporting the spectrum, exporting the spectral library, changing the spectral name, reading the whiteboard file, smoothing the spectral curve, and staggering the spectral curve. Here is a function to read spectral data and spectral header files with MATLAB, as shown in Figure 2.1.

```
>> info = envihdrread('Ironorelibrary.hdr')

info =

包含以下字段的 struct:

    description: ' {ENVI File, Created [Mon Jul 01 16:25:37 2019]}'
      samples: 3375
        lines: 5
         bands: 1
header_offset: 0
   file_type: 'ENVI Spectral Library'
   data_type: 4
  interleave: 'bsq'
 sensor_type: 'Unknown'
  byte_order: 0
wavelength_units: 'Micrometers'
reflectance_scale_factor: 1
   z_plot_range: ' [-0.04, 1.83] '
   band_names: {' Spectral Library' }
spectra_names: {5×1 cell}
   wavelength: [1×3375 double]
```

*Figure 2.1 HDR read function in MATLAB*

It can be found that the number of samples, the number of spectra, the type of data, the unit of wavelength, and the Z-axis range can all be read. The code is shown below.

```
function info = envihdrread(hdrfile)
info=[];
fid = fopen(hdrfile);
[~,name,ext]=fileparts(hdrfile);
if(isequal(fid,-1))
    warnstr=['anddocument ',name,' withdocument ',name,ext,' failed'];
    warndlg(warnstr,'warning');
    return;
end
while true
    line = fgetl(fid);
    if line == -1
        break
    else
        eqsn = findstr(line,'=');
        if ~isempty(eqsn)
            param = strtrim(line(1:eqsn-1));
            param(findstr(param,' ')) = '_';
            value = strtrim(line(eqsn+1:end));
            if isempty(str2num(value))
                if ~isempty(findstr(value,'{')) && isempty(findstr(value,'}'))
                    while isempty(findstr(value,'}'))
                        line = fgetl(fid);
                        value = [value,strtrim(line)];
                    end
                end
                eval(['info.',param,' = "',value,'"'])
            else
                eval(['info.',param,' = ',value,'])
            end
        end
    end
end
fclose(fid);
if(isstruct(info)==0)
    warnstr=[' anddocument ',name,' withdocument ',name,ext,' failed '];
    warndlg(warnstr,'');
    return;
end

if isfield(info,'map_info')
```

```

line = info.map_info;
line(line == '{' | line == '}') = [];
line=textscan(line,'%s','');
line=line{:};
line=strtrim(line);

info.map_info = [];
info.map_info.projection = line{1};
info.map_info.image_coords = [str2num(line{2}),str2num(line{3})];
info.map_info.mapx = str2num(line{4});
info.map_info.mapy = str2num(line{5});
info.map_info.dx = str2num(line{6});
info.map_info.dy = str2num(line{7});
if length(line) == 9
    info.map_info.datum = line{8};
    info.map_info.units = line{9}(7:end);
elseif length(line) == 11
    info.map_info.zone = str2num(line{8});
    info.map_info.hemi = line{9};
    info.map_info.datum = line{10};
    info.map_info.units = line{11}(7:end);
end

xi = info.map_info.image_coords(1);
yi = info.map_info.image_coords(2);
xm = info.map_info.mapx;
ym = info.map_info.mapy;
if yi > 1.5
    ym = ym + ((yi*info.map_info.dy)-info.map_info.dy);
end
if xi > 1.5
    xm = xm - ((xi*info.map_info.dy)-info.map_info.dx);
end

info.x= xm + ((0:info.samples-1).*info.map_info.dx);
info.y = ym - ((0:info.lines-1).*info.map_info.dy);
end

if isfield(info,'pixel_size')
    line = info.pixel_size;
    line(line == '{' | line == '}') = [];
    line=textscan(line,'%s','');
    line=line{:};
    line=strtrim(line);

```

```

        info.pixel_size = [];
        info.pixel_size.x = str2num(line{1});
        info.pixel_size.y = str2num(line{2});
        info.pixel_size.units = line{3}(7:end);
    end
    if isfield(info,'wavelength')
        line = info.wavelength;
        info.wavelength=[];
        line(line == '{' | line == '}') = [];
        line=textscan(line,'%s');
        line=line{:};
        line=strtrim(line);
        for i=1:length(line)
            info.wavelength=[info.wavelength,str2num(line{i})];
        end
    end
    if isfield(info,'fwhm')
        line = info.fwhm;
        info.fwhm=[];
        line(line == '{' | line == '}') = [];
        line=textscan(line,'%s','');
        line=line{:};
        for i=1:length(line)
            info.fwhm=[info.fwhm,str2num(line{i})];
        end
    end
    if isfield(info,'spectra_names')
        line = info.spectra_names;
        info.spectra_names=[];
        line(line == '{' | line == '}') = [];
        line=textscan(line,'%s','delimiter','');
        line=line{:};
        info.spectra_names=line;
    end

    if isfield(info,'group_name')
        line = info.group_name;
        info.group_name=[];
        line(line == '{' | line == '}') = [];
        line=textscan(line,'%s','delimiter','');
        line=line{:};
    end

```

```
info.group_name=line;
```

```
end
```

```
if isfield(info,'classify_spectra')
```

```
    line = info.classify_spectra;
```

```
    info.classify_spectra={};
```

```
    line(line == '{' | line == '}') = [];
```

```
    line=textscan(line,'%s', 'delimiter',',');
```

```
    line=line{:};
```

```
    n=length(line);
```

```
    for i=1:length(line)
```

```
        info.classify_spectra=[info.classify_spectra;str2num(line{i})];
```

```
    end
```

```
end
```

```
if isfield(info,'classify_name')
```

```
    line = info.classify_name;
```

```
    info.classify_name=[];
```

```
    line(line == '{' | line == '}') = [];
```

```
    line=textscan(line,'%s', 'delimiter',',');
```

```
    line=line{:};
```

```
    info.classify_name=line;
```

```
end
```

```
if isfield(info,'group_classify')
```

```
    line = info.group_classify;
```

```
    info.group_classify={};
```

```
    line(line == '{' | line == '}') = [];
```

```
    line=textscan(line,'%s', 'delimiter',',');
```

```
    line=line{:};
```

```
    n=length(line);
```

```
    for i=1:length(line)
```

```
        info.group_classify=[info.group_classify;str2num(line{i})];
```

```
    end
```

```
end
```

```
if isfield(info,'band_names')
```

```
    line = info.band_names;
```

```
    info.band_names=[];
```

```
    line(line == '{' | line == '}') = [];
```

```

line=textscan(line,'%s', 'delimiter',' ');
line=line{:};
info.band_names=line;

```

end

Figure 2.2 shows the reading and display of spectral data using MATLAB.

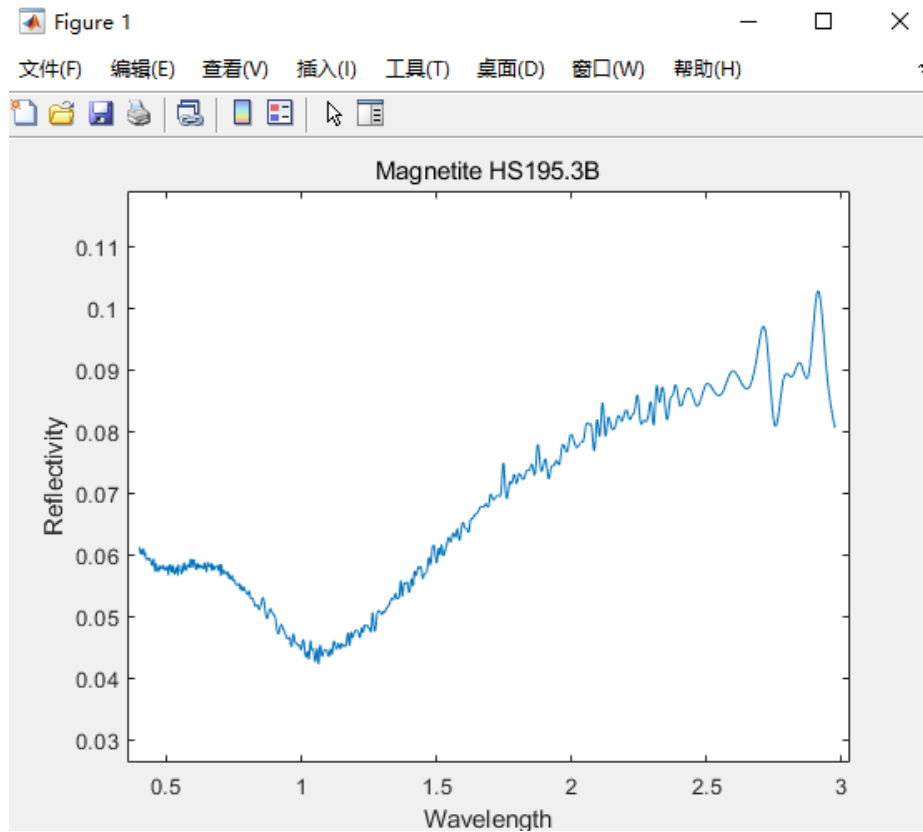


Figure 2.2 Read spectral data and display

The code is shown below.

```

filename=('Magnetite.txt');
a=load(filename);
plot(a(:,1),a(:,2))
xlabel('Wavelength')
ylabel('Reflectivity')
axis([0.3 2.5 0.09 0.135])
title('Magnetite HS195.3B')

```

## 2.2 Iron ore analysis module

The core function of this module is to implement a variety of spectral matching methods used in spectral matching, including spectral angle matching, spectral correlation matching, correlation angle matching, gradient angle matching, discrete information matching, discrete information angle matching, and so on. Below one is an example of a spectral angle calculation.

```
function [errRadians] = hyperSam(a, b)
[p,N] = size(a);
errRadians = zeros(1,N);
for k=1:N
    tmp = a(:,k);
    errRadians(k) = acos(dot(tmp, b)/ (norm(b) * norm(tmp)));
end
return;
```

## 2.3 Iron ore inversion module

Inversions for different iron ores will use different model algorithms. For example, the inversion of magnetite will use the spectral unmixing model. The model mainly calls the unmixing function to realize the function of spectral unmixing, and calculates the unmixed result, inverting the total iron content and error value. The unmixing function mainly includes ATGP algorithm, ICA end element extraction algorithm, ICA component score for calculating correlation, vertex component analysis and pure pixel index algorithm. When the total iron content error of the inversion is large, it is also the pre-processing module adds the function of deriving the reflectance spectrum or the envelope removal function. The inversion model of hematite is mainly a linear regression analysis model. Here are a few of the commonly used unmixing algorithms and their code in MATLAB. Firstly, it is the ATGP algorithm:

```
function [ U, indices ] = hyperAtgp( M, q, Maug )
[p, N] = size(M);
U = [];
indices = [];
c = zeros(N, 1);
for x=1:N
    c(x) = (M(:, x).') * M(:, x);
end
```

```

[dummy, idx] = max(c);
indices = [idx];
U = [M(:,idx)];
start = 1;
if (nargin == 3)
    U = Maug;
end

for n=start:q-1
    P = eye(p) - U * inv(U.' * U) * (U. ');
    for x=1:N
        tmp = (P*M(:, x));
        c(x) = tmp.' * tmp;
    end
    [dummy, idx] = max(abs(c));
    indices = [indices idx];
    U = [U M(:,idx)];
end

```

Secondly, it is the ICA-Endmember extraction algorithm:

```

function [ U, X, n ] = hyperIcaEea( M, q, U_init )
if (ndims(M) ~= 2)
    error('M must be 2d. ');
end

numBands = size(M, 1);
if (nargin == 3)
    [X, U, tmp] = fastica(M, 'numOfIC', q, 'maxNumIterations', 200, ...
        'initGuess', U_init);
elseif (nargin == 2)
    [X, U, tmp] = fastica(M, 'numOfIC', numBands, 'maxNumIterations', 200);
else
    error('Not enough input arguments. ');
end
U = U';
scores = hyperIcaComponentScores(U);
[dummy, idx] = sort(scores, 'descend');
q = min(q, size(U,1));
idx = idx(1:q);
X = X(idx, :);
[val, maxPixels] = max(X. ');
n = maxPixels;
U = M(:, maxPixels);

```



```

if (nargout == 2)
    for i=1:q
        X(i,:) = hyperNormalize(abs(X(i,:)));
    end
end
end

```

```

return;

```

Finally, it is the vertex component analysis algorithm:

```

function [ U, indicies, snrEstimate ] = hyperVca( M, q )
N = size(M, 2);
L = size(M, 1);

rMean = mean(M, 2);
RZeroMean = M - repmat(rMean, 1, N);
[Ud, Sd, Vd] = svds(RZeroMean*RZeroMean.'/N, q);
Rd = Ud.*(RZeroMean);
P_R = sum(M(:).^2)/N;
P_Rp = sum(Rd(:).^2)/N + rMean.*rMean;
SNR = abs(10*log10( (P_Rp - (q/L)*P_R) / (P_R - P_Rp) ));
snrEstimate = SNR;

```

```

fprintf('SNR estimate [dB]: %g\n', SNR);

```

```

SNRth = 15 + 10*log(q) + 8;

```

```

if (SNR > SNRth)
    d = q;
    [Ud, Sd, Vd] = svds((M*M.')/N, d);
    Xd = Ud.*M;
    u = mean(Xd, 2);
    Y = Xd ./ repmat( sum( Xd .* repmat(u,[1 N]) ),[d 1]);

```

```

else
    d = q-1;
    r_bar = mean(M.').';
    Ud = pca(M, d);
    R_zeroMean = M - repmat(r_bar, 1, N);
    Xd = Ud.' * R_zeroMean;
    c = zeros(N, 1);
    for j=1:N
        c(j) = norm(Xd(:,j));
    end
    c = repmat(max(c), 1, N);
    Y = [Xd; c];

```

```

end
e_u = zeros(q, 1);
e_u(q) = 1;
A = zeros(q, q);
A(:, 1) = e_u;
I = eye(q);
k = zeros(N, 1);
for i=1:q
    w = rand(q, 1);
    tmpNumerator = (I-A*pinv(A))*w;
    f = tmpNumerator / norm(tmpNumerator);

    v = f.'*Y;
    k = abs(v);
    [dummy, k] = max(k);
    A(:,i) = Y(:,k);
    indices(i) = k;
end
if (SNR > SNRth)
    U = Ud*Xd(:,indices);
else
    U = Ud*Xd(:,indices) + repmat(r_bar, 1, q);
end
return;

function [U] = pca(X, d)
    N = size(X, 2);
    xMean = mean(X, 2);
    XZeroMean = X - repmat(xMean, 1, N);
    [U,S,V] = svds((XZeroMean*XZeroMean.)/N, d);
return;

```

For the case where the unmixing is nonlinear, we need to perform the derivation or envelope removal. The envelope removal is obtained by comparing all the maximum points on the spectrum and then obtaining the maximum value. Then, using the maximum point as an endpoint of the envelope, the slope of the line connecting the maximum value of the point with the wavelength growth direction is obtained, and the point with the largest slope is used as the next end point of the envelope. Next, the point of the maximum value is used as the break point of the envelope, and the same calculation as the second part is performed in the direction of decreasing wavelength until the starting point on the curve. Finally, the envelope of all the breakpoints is

connected to form the curve, and the actual spectral reflectance is used to divide the reflectance of the corresponding band on the envelope to obtain the result. Taking the magnetite spectral curve as an example, the result of the envelope removal is as follows.

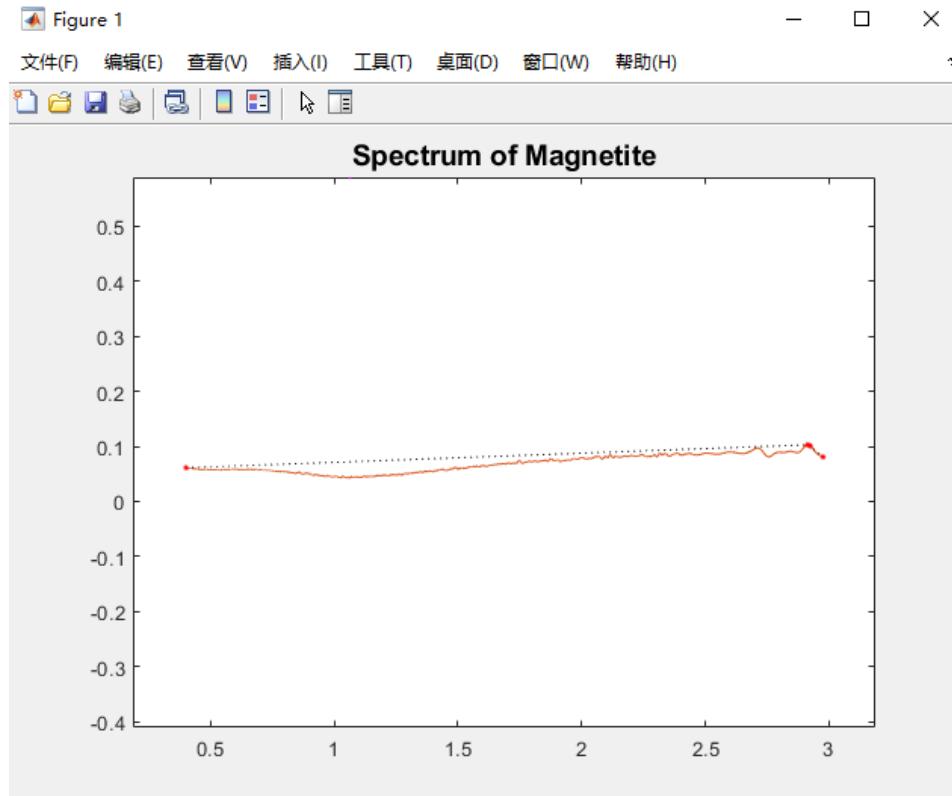


Figure 2.3 Envelope removal result

The envelope removal code is as follows:

```
[WaveLength,Orig_Spectrum]=textread('Magnetite.txt','%f%f','headerlines',3);
x=WaveLength;
y=Orig_Spectrum;
len=length(x);
i=1;
k=1;
tempWav(k)=x(i);
tempRef(k)=y(i);
flag_i=1;
while(i<=len & flag_i)
    if i==len
        break;
    end
    j=i+1;
```

```

flag_j=1;
while(j<=len & flag_j)
    if j==len
        k=k+1;
        tempWav(k)=x(j);
        tempRef(k)=y(j);
        flag_i=0;
        break;
    end
    m=j+1;
    while(m<=len)
        if m==len
            k=k+1;
            tempWav(k)=x(j);
            tempRef(k)=y(j);
            i=j;
            flag_j=0;
            break;
        else
            A=[x(i),1;x(j),1];
            b=[y(i);y(j)];
            X=inv(A)*b;
            y1(m)=X(1)*x(m)+X(2);
            if y1(m)<y(m)
                j=j+1;
                break;
            else
                m=m+1;
                continue;
            end
        end
    end
end
end

wav1=x;
ref1=interp1(tempWav,tempRef,wav1);
plot(x,y)
hold on
plot(wav1,ref1,'k')
plot(tempWav,tempRef,'r.')
wav=wav1;
ref=y./ref1;
plot(wav,ref,'m')

```

```
title('Spectrum of Magnetite','fontsize',14,'fontweight','b')
legend('Spectrum of Origin ','Envelope','Envelope Node','Spectrum of Envelope Removing',3)
xlabel('wavelength(\num)','fontsize',12,'fontweight','b')
ylabel('Reflectance(%)','fontsize',12,'fontweight','b')
```

### 3 Spectral Characteristics Analysis of Iron Ore

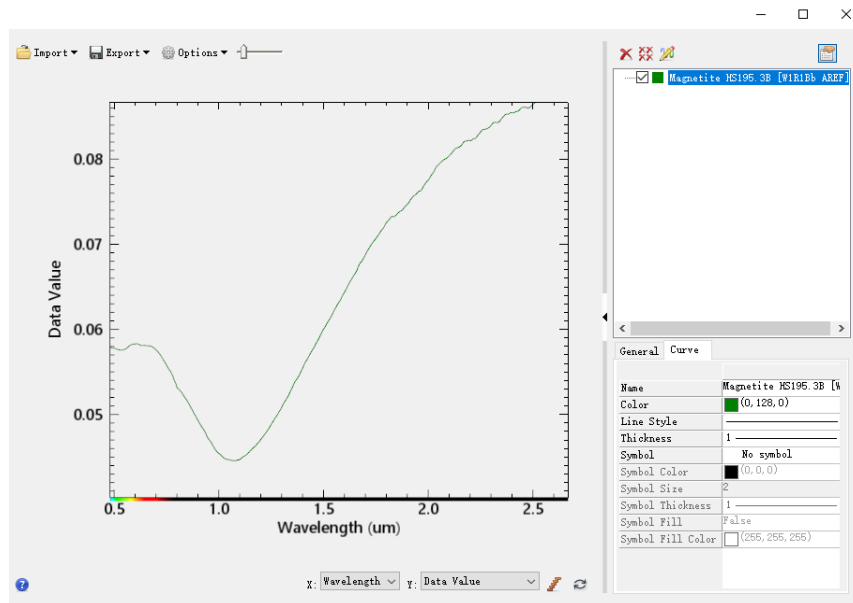
For the analysis of the spectral characteristics of iron ore, the most widely used application is spectral identification matching, that is, the model is based on the iron ore spectral library to test the iron ore type of an unknown spectrum. So, I first need to build a spectral library and use a detected spectrum to verify the matching identification method. Before the establishment of the iron ore spectral library, the spectral properties of each iron ore should be studied first.

#### 3.1 Spectral characteristics of iron ore

The spectral characteristics of iron ore are related to the type of iron ore. The spectral characteristics of different types of iron ore are not the same, and the same kind of iron ore interference components have different spectral characteristics. But there are similarities between them.

##### 3.1.1 Spectral characteristics analysis of magnetite

Magnetite is also an iron ore that is mainly studied in this report. It is mainly composed of  $\text{Fe}_3\text{O}_4$ . It belongs to the equiaxed crystal system, and the crystal exhibits an octahedron or a dodecahedron. The surface of the crystal has various stripes, and the streaks are black, mostly granular agglomerates. Its body color is grayish black, and some are also dark blue, with a semi-metallic luster and very low transparency. The fracture surface of the ore is uneven, and its hardness is between 5.5 and 6.5, and the density is between 5.1 and 5.2 g/cm<sup>3</sup>. It has very strong magnetic properties, a fragile structure, and is odorless and tasteless. Often produced in magmatic rocks and metamorphic rocks. The spectral information of the magnetite extracted from the USGS library is shown in figure 3.1.



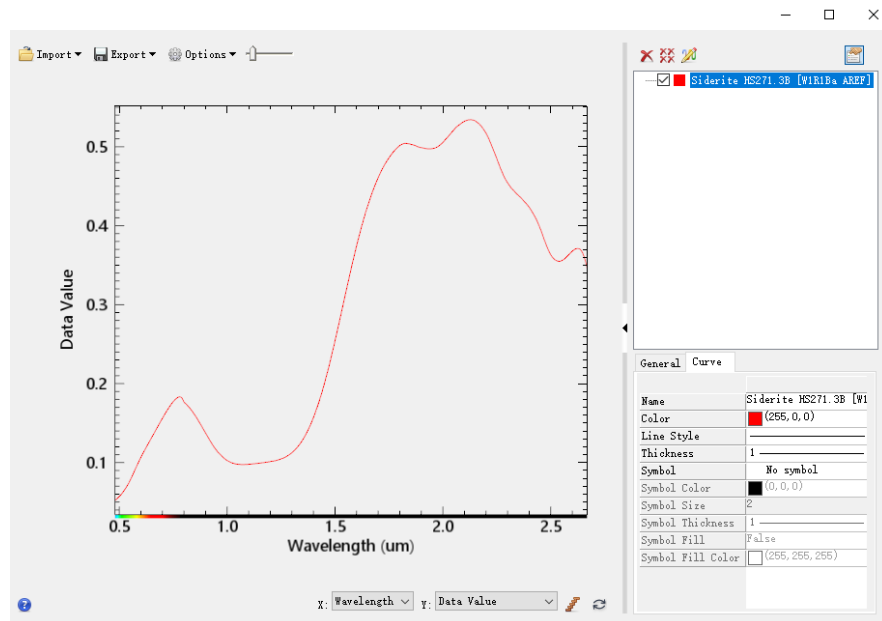
*Figure 3.1 Magnetite spectral characteristic curve*

As can be seen from figure 3.1, the spectral reflection curve of magnetite is a relatively smooth curve, with no obvious reflection peaks and absorption valleys from 0.5 $\mu\text{m}$  to 1.0 $\mu\text{m}$  and 1 $\mu\text{m}$  to 2.6 $\mu\text{m}$ , but a slight at 0.5 $\mu\text{m}$ . The absorption basin may be related to the strong absorption of cyan light by magnetite. There is a strong absorption valley at 1 $\mu\text{m}$  due to the absorption of magnetite to the near infrared. The spectral reflectance of magnetite increases with increasing wavelength.

### 3.1.2 Spectral characteristics analysis of siderite

The main components of siderite are 2%  $\text{FeCO}_3$ , 60%  $\text{FeO}$  and 38%  $\text{CO}_2$ . Its iron content is very high, about 50%, and does not contain other impurities such as phosphorus or sulfur. Zinc, magnesium and manganese are often used to replace iron, and are made into solid solution such as siderite-rhombic, siderite-magnesite and siderite-magnesium. In addition, the siderite often contains cobalt and calcium. The shape of the siderite is a trigonal crystal, the crystal is rhomboid, and the crystal plane

is relatively curved. Agglomerates are granular, massive, tuberculous, grape-like, and earthy. Granular globules are called globular siderite, and cryptocrystalline gelatinous siderite is called melamine. The spectral information of the siderite extracted from the USGS library is shown in figure 3.2.



*Figure 3.2 Siderite spectral characteristic curve*

The spectral curve of the siderite and the spectral curve of the plant are somewhat similar, but not identical, except that the approximate shape of the curve, and the reflectance characteristics are different on different wave ranges. The spectral reflection curve of siderite has a reflection peak at  $0.8\mu\text{m}$ , indicating that the siderite has a strong absorption effect on red light. It indicates that as the wavelength increases, the reflectivity gradually decreases and maintains a level at a wavelength of  $1\mu\text{m}$  up to a wavelength of  $1.4\mu\text{m}$ , indicating that the siderite has a strong absorption effect on near-infrared light. In the range of  $1.3\mu\text{m}$ - $3\mu\text{m}$ , short-wave infrared, there is a distinct



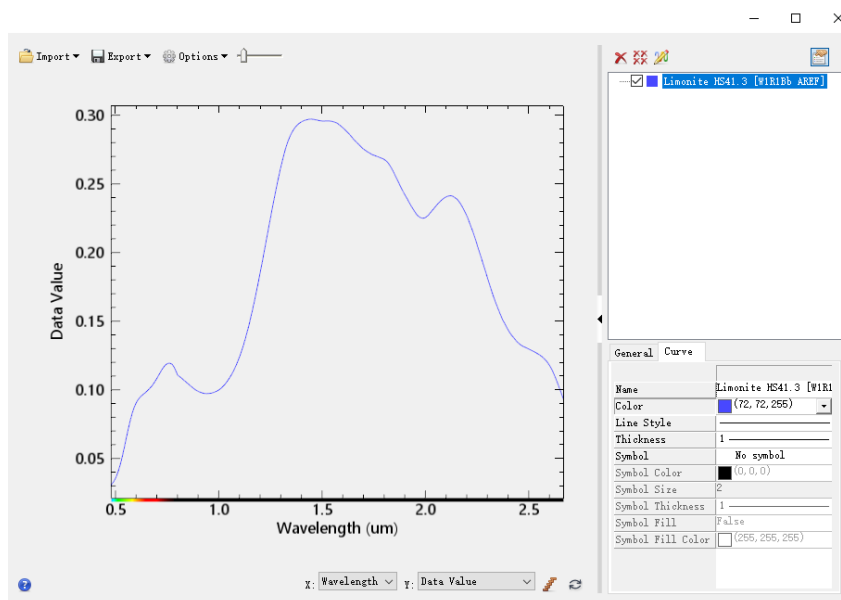
reflection peak, that is, there are three absorption valleys at 1.9 $\mu\text{m}$ , 2.3 $\mu\text{m}$  and 2.9 $\mu\text{m}$ , which may be due to some impurity pairs in siderite. The above three wavelengths are strongly absorbed. When the thickness is  $>2.7\mu\text{m}$ , the reflectivity drops sharply, indicating that the siderite has a strong absorption to the mid-infrared.

### 3.1.3 Spectral characteristics analysis of limonite

The main component of limonite is  $\text{Fe}_2\text{O}_3 \cdot n\text{H}_2\text{O}$ , and the iron content is about 35%. In fact, it is not a single-component iron ore, but an agglomerate of iron hydroxide such as goethite and agglomerates of hydrous silica and shale and the composition is very diverse. It is usually lumpy, earthy, stalactite, loosely porous, powdery or grape-like. The color is generally tan or dark brown, including streaks. The surface of the ore is dim, the hardness varies with its composition and morphology, the hardness of limonite with a high silicon content is as high as 5.5, and the hardness of the clay-like limonite rich in mud is as low as 1. It is formed by oxidative decomposition of iron-containing minerals, especially in the surface parts rich in metal sulfides. Ore is often exposed to limonite after exposure to air and oxidation. In addition, the limonite deposits formed by lakes and marshes tend to accumulate large amounts, and they can be used as raw materials for iron making. Limonite belongs to the weathering product of iron-containing minerals ( $\text{Fe}_2\text{O}_3 \cdot n\text{H}_2\text{O}$ ), and its performance is highly affected by the content of water.

The limonite deposit is an acid-bearing ore-forming contact with limestone to form a pyrite iron cap-like limonite deposit. Most of the whole deposit is composed of limonite ore and quartz, of which quartz accounts for 10-40%. The more quartz stone, the less

limonite, and vice versa. The spectral information of the limonite extracted from the USGS library is shown in figure 3.3.



*Figure 3.3 Limonite spectral characteristic curve*

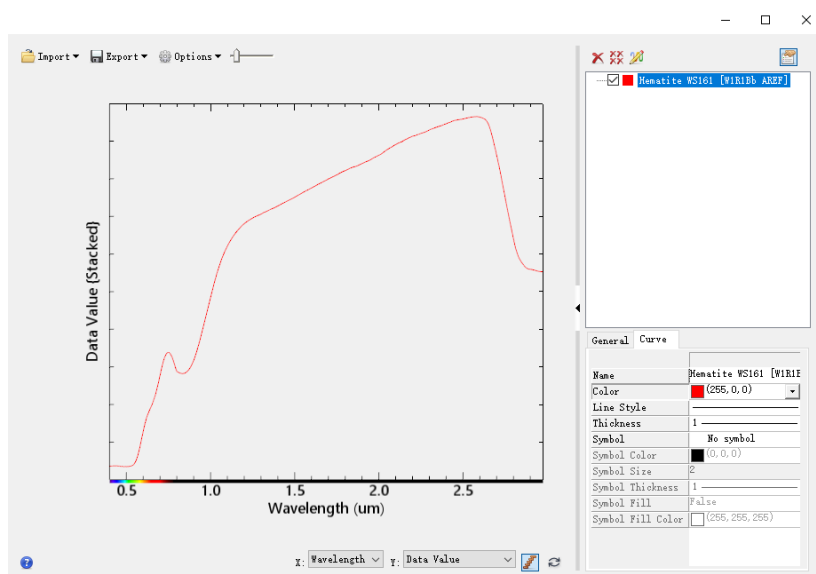
The characteristics of the reflection curve of limonite are similar to those of siderite, but the absorption characteristics of different electromagnetic radiation are different. There is a reflection peak between 0.7 $\mu$ m and 0.8 $\mu$ m, which is due to the strong reflection of limonite on red light. The absorption valley of 0.8 $\mu$ m to 1.3 $\mu$ m indicates that limonite has a strong absorption effect on the near infrared. Like siderite, limonite also has a relatively high reflectivity for short-wave infrared and a valley of absorption at 2 $\mu$ m.

#### 3.1.4 Spectral characteristics analysis of hematite

The main component of hematite is  $\text{Fe}_2\text{O}_3$ , and its crystal structure is an oxide mineral of hexagonal crystal. It is consistent with the crystal axis of maghemite, which is a phenomenon of homogeneity. Its single crystal is usually diamond or strip. The

shape of the agglomerates is flaky, scale-like, granular, scorpion-like, kidney-like, earthy, dense, and so on. The color is reddish brown, gray and pure black, and the streaks are rust red. The gloss is between metal and semi-metal. The hardness range is around 6.

Agglomerates of metallic luster flake hematite are called specular hematite. The metallic lustrous scaly hematite agglomerates are called mica hematite. Hematite-like hematite is called scorpion hematite. It can be seen that hematite is a widely distributed iron ore in nature, and is also an important ironmaking raw material, which can be used as a pigment in the art field. The spectral information of the hematite extracted from the USGS library is shown in Figure 3.4.



*Figure 3.4 Hematite spectral characteristic curve*

Like other iron ores, hematite also has a distinct reflection peak at the red band (0.7 $\mu$ m-0.8 $\mu$ m), and the near-infrared absorption intensity increases, and the reflectance reaches a peak at the short-wave infrared.

### 3.1.5 Spectral characteristics analysis of goethite

Goethite is often distributed near mud marshes and is widely distributed. The rust on the rusty iron ore is composed of goethite. In general, the chemical action of water and iron ore in the presence of oxygen produces goethite. Its color is yellowish brown or red, and the crystal structure is mainly in the form of flakes, columns or needles, so the structure of goethite is relatively loose, and the hardness is very low.

There is also a large amount of goethite in the seabed or at the bottom of the lake. It is very important for the industrial field, and iron and industrial pigments will use goethite. The spectral information of goethite extracted from the USGS library is shown in Figure 3.5.

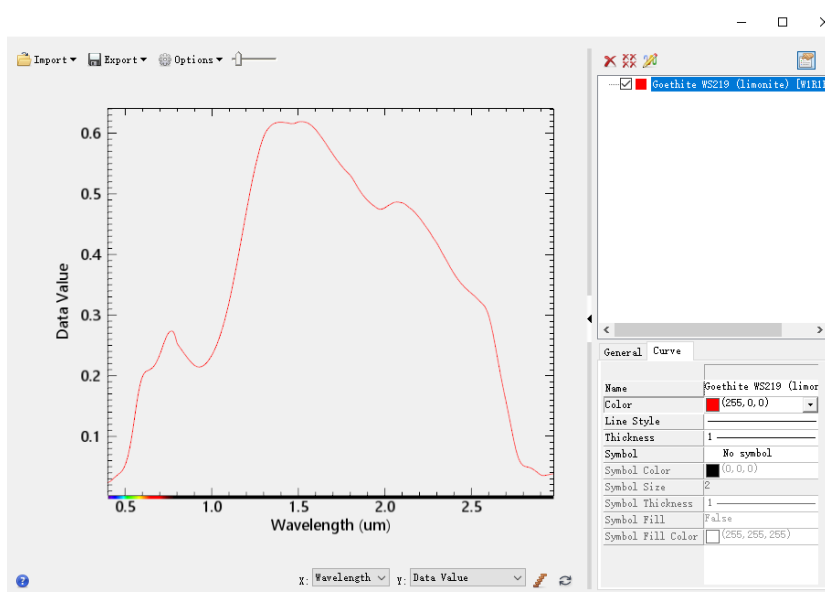


Figure 3.5 Goethite spectral characteristic curve

The spectral characteristic curve of goethite is almost identical to that of limonite, but the overall reflectivity is about 0.2-0.3 higher than that of limonite.

### 3.1.6 Comparison of spectral curves of different iron ores

Each iron ore has its own spectral characteristic curve, but there are similarities and similarities between them. As shown in Figure 3.6, all iron ore has a reflection peak between  $0.7\mu\text{m}$  and  $0.8\mu\text{m}$ , and there are obvious reflection bands in the short-wave infrared band, and the reflectance in the mid-infrared band drops to less than 0.1. The absorption band of siderite is shorter than other minerals, which occurs from  $1.7\mu\text{m}$ , while other minerals start from  $1.3\mu\text{m}$ . The reflectivity range of magnetite and hematite is relatively small compared to the other three iron ore.

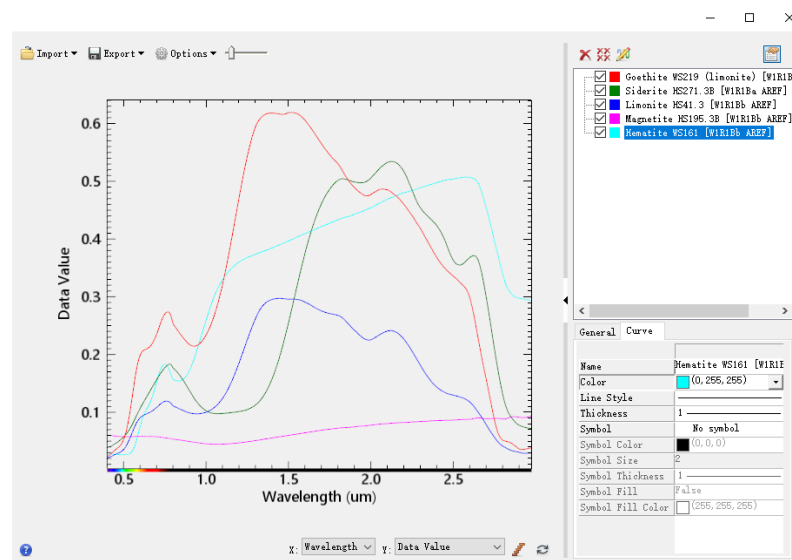


Figure 3.6 Comparison of spectral curves of different iron ores

### 3.2 Iron ore species identification analysis

After studying the spectral characteristics of various iron ores, it is necessary to start looking for a qualitative analysis method for the type of iron ore, namely spectral matching. Spectral matching method is a method for judging and recognizing the types of ground objects by remote sensing images. The similarity of two spectral curves is

used to judge the types of features. There are two types of spectral matching: one is to compare the spectral spectrum of the sample with the spectral curve in the spectral library; the other is to classify the spectral response curve itself between the sample and the sample.

There are many methods for spectral matching, the most typical of which is spectral angle matching, which is to calculate the similarity value between them by calculating the angle value between a sample pixel spectrum and a reference spectrum, so in actual processing I choose the method of spectral angle matching.

### 3.2.1 Data and sample spectra

The experimental data is from the Nanshan Iron Mine in Maanshan City, Anhui Province. It is known that this sample is a mixture of two different grades of magnetite. Its spectrum is shown in figure 3.7. It can be found that if the composition of the sample is unknown, it is difficult to judge the specific type of the iron ore only by the naked eye, so it is necessary to use the spectral matching method to judge.

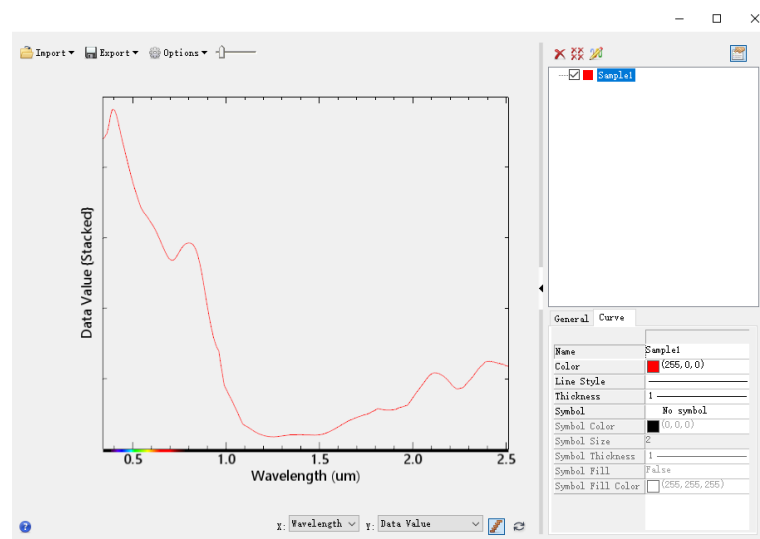


Figure 3.7 Spectral curve of sample 1

### 3.2.2 Result and analysis

The spectral angle matching method is used to verify the type of the mixed sample. Figure 3.8 is the process interface for selecting the weights of the three matching methods before matching. The weight of the selected spectral angle matching is 1, and the matching spectral library is obtained from the previous step that based on the iron ore spectral library created by the USGS.

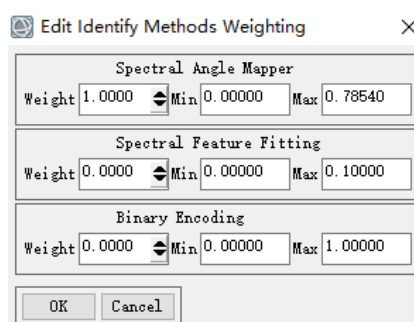


Figure 3.8 Spectral matching method uses SAM method

The matching results show that the two iron ores with the highest similarity are magnetite, their fractions are 0.657 and 0.560 respectively, and we know that the sample is magnetite, so the matching result is correct. The detailed results are shown in figure 3.9.

The image shows a window titled "Spectral Analyst" with a menu bar (File, Options) and a table of results. The table has three columns: "Unknown: Sample1", "Library Spectrum", "Score", and "SAM". The data rows list various iron ore samples and their corresponding scores and SAM values.

Unknown: Sample1	Library Spectrum	Score	SAM
	Magnetite HS78.3B [W	[0.657]	{0.657}
	Magnetite HS195.3B [	[0.560]	{0.560}
	Hematite GDS69.a 150	[0.527]	{0.527}
	Hematite GDS69.b 104	[0.470]	{0.470}
	Hematite HS45.3 [W1R	[0.460]	{0.460}
	Hematite GDS69.c 60-	[0.393]	{0.393}
	Hematite GDS69.d 30-	[0.276]	{0.276}
	Goethite WS219 (limo	[0.238]	{0.238}
	Limonite HS41.3 [W1R	[0.226]	{0.226}
	Hematite GDS69.e 20-	[0.214]	{0.214}
	Pitch Limonite GDS10	[0.201]	{0.201}
	Hematite FE2602 [W1R	[0.186]	{0.186}
	Hematite WS161 [W1R1	[0.170]	{0.170}
	Hematite GDS27 [W1R1	[0.137]	{0.137}
	Hematite GDS69.f 10-	[0.129]	{0.129}
	Siderite HS271.3B [W	[0.115]	{0.115}
	Hematite GDS69.g <10	[0.095]	{0.095}

Figure 3.9 Spectral angle matching method matching result

## **4 Inversion of total iron content of magnetite**

In general, most of the current inversion of total iron content in magnetite is achieved using chemical methods, namely potassium dichromate titration. With the update of technology, there are more methods that are more advantageous in some respects, such as hyperspectral spectral unmixing technology to invert the total iron content; after decomposing, a number of mixed pixels can be obtained and after obtaining the ratio of these endmembers, the value of the iron element can be calculated. Furthermore, the XRF method can also directly measure the iron content, but because of the low precision, it can only be temporarily used as a method of auxiliary verification.

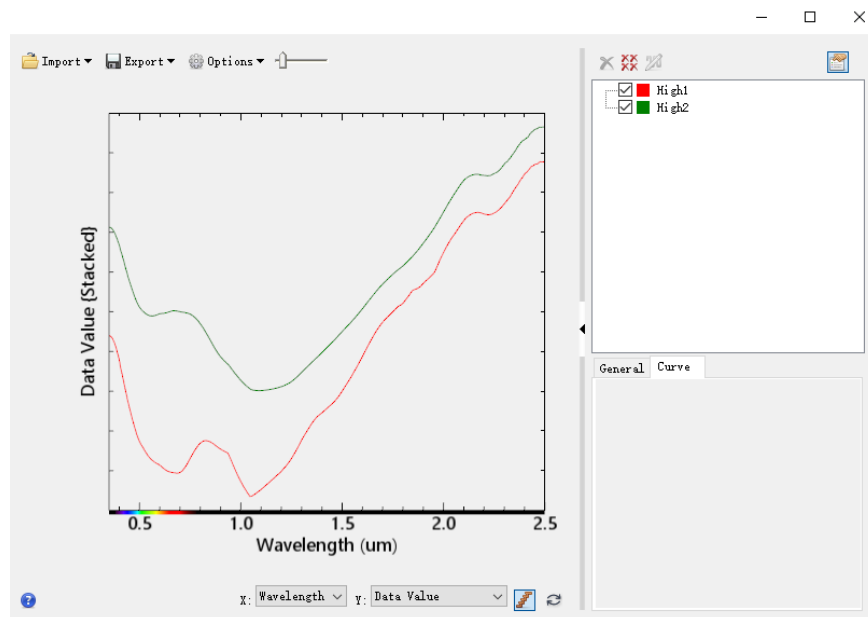
### **4.1 Retrieving total iron content based on spectral unmixing**

Although at the present stage, the inversion of total iron content of magnetite is generally determined by potassium dichromate titration, and when the accuracy of the content is not high, the spectrometric determination of total iron content is simpler, faster and more secure than traditional chemical methods.

#### **4.1.1 Data introduction**

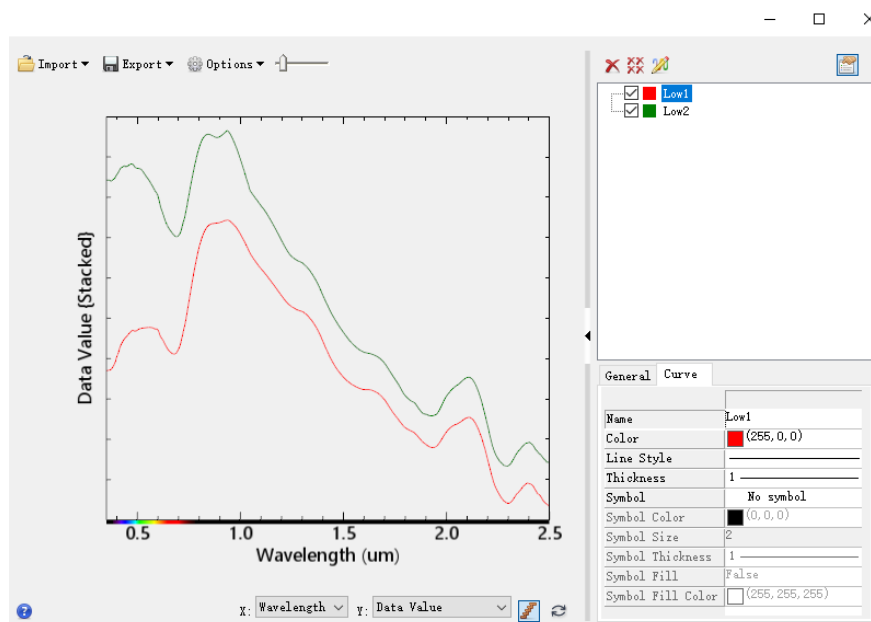
The sample is still obtained from the Nanshan iron ore mine in Maanshan. Among them, High1 and High2 are two magnetite samples with higher total iron content and higher grade. Their calibration total iron content is 64.51% and 63.26% respectively. Their spectral are shown below.





*Figure 4.1 Two high-grade sample spectral curves*

Low1 and Low2 are two magnetite samples with low total iron content and low grade, and their total iron content is 19,45% and 18.85% respectively. Their spectral are shown below.



*Figure 4.2 Two low-grade sample spectral curves*

#### 4.1.1 Method and Result analysis

Combine their spectral curves as shown in Figure 4.7. It can be found that the reflectance of the overall spectral curve of the two samples High1 and High2 with higher total iron content is smaller than Low1 and Low2. It shows that the higher the total iron content of magnetite, the lower the spectral reflectance.

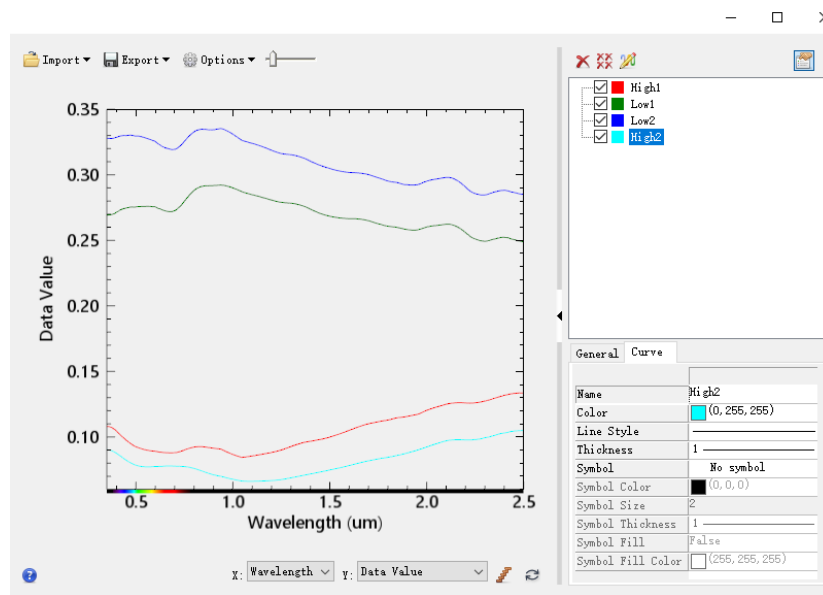
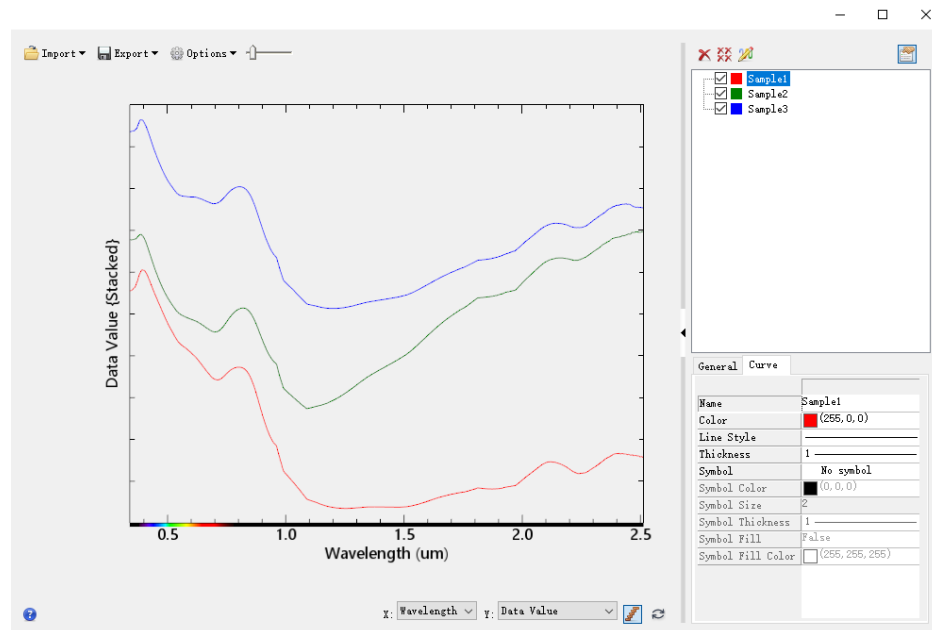


Figure 4.3 Two kinds of sample spectral curves

The spectral characteristics of magnetite with different iron content also have similarities and differences. They all have an absorption valley at  $0.7\mu\text{m}$  and  $1\mu\text{m}$ , but the magnetite with higher total iron content increases with the increase of wavelength after  $1\mu\text{m}$ , and the magnetite with lower total iron content is  $1\mu\text{m}$ . As the wavelength increases, the reflectivity decreases, and they show different trends.

The spectra of the mixed pixels were also collected in the experiment. The three spectral curves shown in figure 4.4 are respectively sample1 which contains 70% Low1 and 30% High1, the sample2 which contains 30% Low1+70% High1, and sample3

which contains 50% Low2+50 % High2. The reflectance of the three spectral curves decreases with the increase of the content of high total iron content of magnetite, which further indicates that the total iron content has an influence on the spectral characteristics of magnetite.

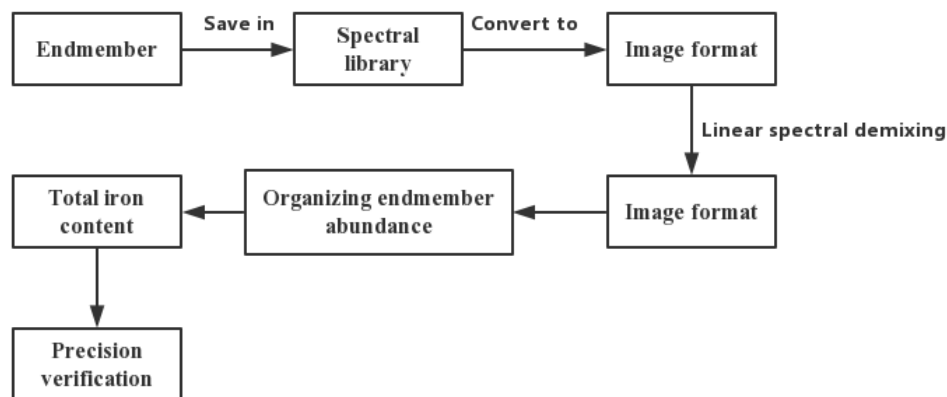


*Figure 4.4 Three kinds of mixed sample spectral curves*

The total iron content was determined by spectral unmixing method. In the experiment, the total iron content of the 4 sample iron ore was known to be mixed with each other in different proportions, and their spectral curves were measured, and then the spectra were mixed. Pixel decomposition can result in a linear result (the percentage of each component obtained by decomposition is approximately or unchanged), or a non-linear result (the percentage of each component obtained by spectral unmixing is different from the mixing ratio and varies greatly). If it is a linear result, the total iron content of the mixed sample can be calculated directly from the percentage of total iron

content of the component and the percentage of the mixed sample. For nonlinear results, the spectrum needs to be derivatized or the envelope removal algorithm is processed to achieve a linearity of the spectrum, and then the accuracy is verified.

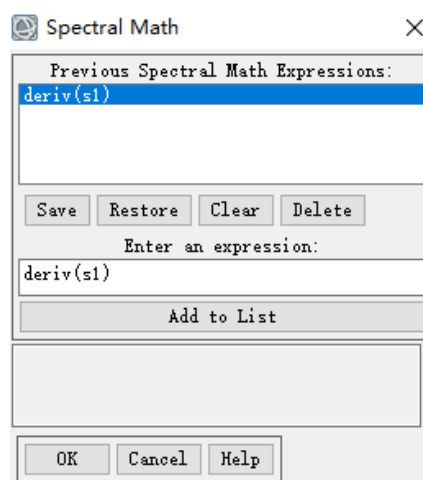
The forward solution can calculate the difference between the total iron content of the actual sample and the total iron content calculated by the unmixing result and obtain a relatively accurate rule by verifying the regularity of the samples of the plurality of sets of known mixing ratios. Iron content inversion method can be obtained by manually mixing the spectra of the two magnetite samples, comparing the spectra of the samples mixed according to their ratios, and quantifying the difference law, and also obtaining the approximate true total iron content. Its approximate technical route is shown in figure 4.5.



*Figure 4.5 Workflow of total iron content*

The following three spectral samples are spectrally unmixed. First, the spectral files of the three mixed samples are separately converted into the format of the ENVI image.

The purpose of this step is to make it accessible for the the linear spectral unmixing tool that comes from ENVI5.3. After processing, the Convert Library to Image tool in the VIPER toolbox is used here, and the image file is opened with ENVI5.3 after conversion. After obtaining the image file of the mixed spectrum, two endmember spectral libraries are created, one is the original end element spectrum, and the other is the endmember spectrum after derivation. The derivative spectrum has unique advantages in spectral analysis. There are three main points. The first one is that it can improve the resolution of the spectrum, extract the respective reflection peaks from the overlapping reflection spectra and perform quantitative analysis separately. Secondly, it can reduce the influence of background absorption. For those cases where the background influence is more serious, the quantitative analysis can also be performed relatively accurately by derivative spectroscopy. Finally, the derivative spectroscopy can accurately determine the specific position of the absorption peak and can improve the signal-to-noise ratio and detection sensitivity. The function for deriving the spectrum is shown in figure 4.6.



*Figure 4.6 Use the Spectral Math tool*

The spectra of the three mixed pixels and the endmember spectra are derived as figure 4.7 and 4.8.

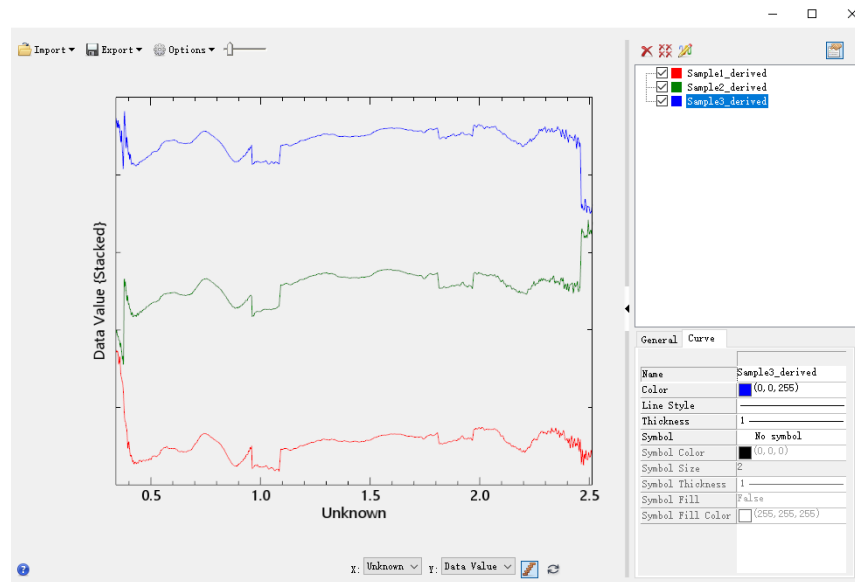


Figure 4.7 Derived mixed sample spectral

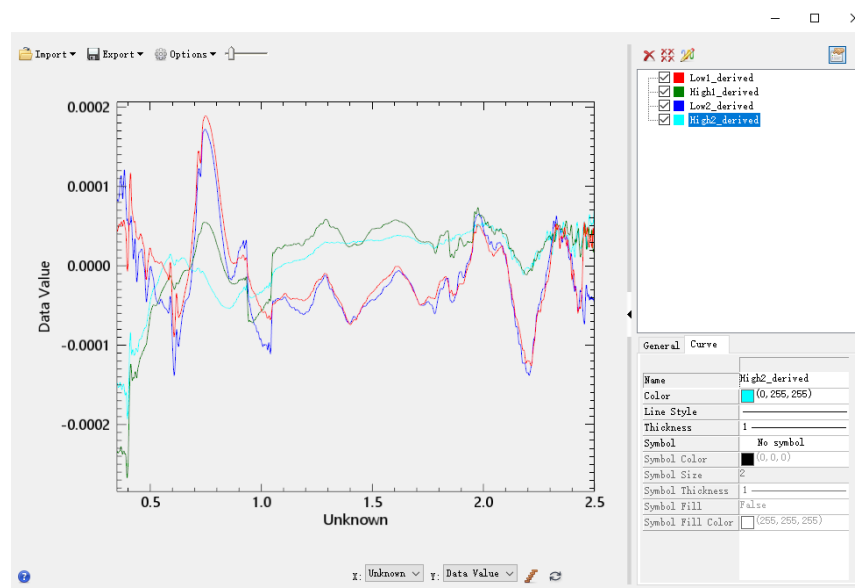


Figure 4.8 Derived 4 sample spectral

The spectral spectroscopic unmixing of the spectra was performed using the Linear Spectral Unmixing tool to obtain the endmember spectral content. All samples are

known to be 4ml. Table 4.1 below shows the results of reflectance spectral unmixing.

After the unmixing ratio is obtained, we need to calculate the true total iron content and the measured total iron content. The formula is as follows:

$$a = \frac{\rho_1 * V_1 * i_1 * m_1 + \rho_2 * V_2 * i_2 * m_2}{\rho_1 * V_1 * m_1 + \rho_2 * V_2 * m_2}$$

Where:  $a$  - percentage of total iron content,  $\rho_1$  - the density of the first end sample, g/ml,  $\rho_2$  - the density of the second end sample is g/ml,  $V_1$  - the volume of the first endmember sample ml,  $V_2$  - the volume of the second endmember sample ml,  $i_1$  - the mixing ratio of the first end-element sample,  $i_2$  - the mixing ratio of the second endmember sample,  $M_1$  - the total iron content of the first endmember sample,  $M_2$  - the total iron content of the second endmember sample

The English abbreviation for Root Mean Square is RMS, which means root mean square error, that is, the effective value can be simply described as the degree of dispersion of the sample, and also the square root of the average of the square of a set of statistics. Its calculation formula is as follows:

$$\sqrt{((X_1^2 + X_2^2 + X_3^2 + \dots + X_n^2) / n)}$$

Where:  $X_i$  — the difference between the measured value and the comparison value of the  $i$ th sample,  $n$  — the number of samples measured.

*Table 4.1 Reflectivity unmixing result*

Name	Endmember sample quality and mixing ratio	Ratio after unmixing	True total iron content	Measured total iron content	RMS
Sample1	70% Low1 (5.202g) + 30%High1 (3.337g)	50.8% and 22.1%	37.1%	33.3%	0.09

Sample2	30% Low1 (2.230g) + 70%High1 (7.787g)	11.9% and 64.2%	54.5%	59.55%
Sample3	50% Low2 (3.326g) + 50%High2 (5.174g)	9.8% and 79.1%	45.8%	60%

I found that the result of the unmixing can be judged to be nonlinear, because the ratio after the unmixing is far from the true mixing ratio, so the algorithm for deriving the reflectance spectrum or the algorithm of envelope removal is needed. The method of guidance is also mentioned above. The results of the unmixing after derivation are shown in table 4.2 below.

*Table 4.2 Derived spectral unmixing result*

Name	Endmember sample quality and mixing ratio	Ratio after unmixing	True total iron content	Measured total iron content	RMS
Sample1	70%Low1 (5.202g) + 30%High1 (3.337g)	72.7% and 27.3%	37.1%	35.66%	0.06
Sample1	30%Low1 (2.230g) + 70%High1 (7.787g)	27.1% and 72.9%	54.5%	55.6%	
Sample1	50%Low1(3.326g) + 50%High1 (5.174g)	22.7% and 78.3%	45.8%	56.31%	

After the derivation process, the ratio of the unmixed is basically similar to the true ratio, and the total iron content is also more accurate, especially for the unmixing of Low1 and High1, and the true total iron content is almost one percentage point worse. For the unmixed results of the Low2 and High2 mixed samples and the true total iron content, I conjecture that it may be related to their endmember spectra to eliminate the influence of each other by derivation and I will try the envelope removal algorithm in the future.

## 4.2 XRF method assists in verifying iron content



The full name of the XRF method is X-ray fluorescence spectrometry. The secondary X-rays generated by X-ray irradiation on the sample to be tested are called X-ray fluorescence, and the irradiated X-rays are called primary X-rays. The XRF instrument consists of an X-ray tube and a probe. The incoming radiation wrapped by the XRF instrument is called an X-ray, which can effectively excite the sample to be tested. Each element in the excited sample emits another ray, a secondary X-ray. The secondary X-rays emitted by different elements have different energy spectral characteristics. The probe collects the energy and spectral information of these reflected secondary X-rays. Then, through the designed instrument software, the information collected by the detection system is converted into the types and contents of various elements in the sample. This method can in principle measure every element after the element in the periodic table.

This method has the advantage of faster analysis than the traditional chemical method. The measurement precision affects the measurement time, and generally all the measurements of the sample can be completed in less than ten minutes. This method does not require the state of the object to be measured, and the solid liquid state can be measured, and the sample is not destroyed during the measurement. Although the measurement accuracy is not as high as the chemical method, this method can be used to obtain a total iron content and accurately invert it to ensure accuracy.

However, this method also has certain limitations. First, its sensitivity to light elements is low, and the measured iron element results are susceptible to elemental interference and superimposed peaks. Table 4.3 below shows the results of the

measurements on the samples High2 and Low2, which can be seen to be similar to the chemical methods. Using this method, we can verify the accuracy of the total iron content obtained by spectroscopy or chemical methods.

*Table 4.3 XRF verification result*

<b>Name</b>	<b>Iron content measured by XRF</b>	<b>Iron content determined by chemical method</b>	<b>RMS</b>
Low2	17.366%	18.85%	0.02
High2	65.521%	63.26%	

## 5 Conclusion

From the practical application, this report establishes a preliminary framework for a spectroscopic analysis system for iron ore. From the qualitative analysis of the spectral matching angle of various types of iron ore to the quantitative analysis of the spectral unmixing angle of magnetite, the preliminary application of the iron ore analysis method was designed.

Regards to systems, a combination of software modules can perform basic iron ore analysis. The software module uses MATLAB to call the function model, which can complete the three major modules of the software system, including basic data preprocessing module, matching identification qualitative analysis module and total iron content inversion quantitative analysis module.

For qualitative analysis, these iron ores can be further understood by analyzing the spectrum of each iron ore, and these analyses are prepared for the theoretical basis of subsequent spectral matching recognition. A matching benchmark can be provided for matching identification by constructing an iron ore spectral library. The matching recognition is mainly applied to the spectral angle matching model algorithm, and the results of matching the samples are completely consistent with the real situation.

Finally, the quantitative analysis is the core part of this report. The full iron content inversion process not only provides accurate total iron content for most samples, but also allows for an assessment of accuracy. This is faster, easier, simpler, and less

expensive than traditional chemical potassium dichromate titration. This design also uses the XRF ray method to aid in verification accuracy.

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