Retrieving Volume FeO and TiO$_2$ Abundances of Lunar Regolith with CE-2 CELMS Data using BPNN Method

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Abstract. The volume FeO and TiO$_2$ abundances (FTAs) of lunar regolith will be more important to understand the geological evolution of the Moon compared to the optical and gamma-ray results. In this paper, the volume FTAs are retrieved with the microwave sounder (CELMS) data from Chang’E-2 satellite using the back propagation neural network (BPNN) method. Firstly, a three-layered BPNN network with five-dimension input is constructed by taking nonlinearity into account. Then, the brightness temperature ($T_B$) and surface slope are set as the inputs and the volume FTAs are set as the outputs of the BPNN network. Thereafter, BPNN network is trained with the corresponding parameters collected in Apollo, Luna, and Surveyor missions. Finally, the volume FTAs are retrieved with the trained BPNN network using the four-channel $T_B$ concluded from the CELMS data and the surface slope estimated from LOLA data. The rationality of the retrieved FTAs is verified by comparing with the Clementine UV-VIS results and LP-GRS results. The retrieved volume FTAs enable us to re-evaluate the geological features of the lunar surface. Several important results are as follows. Firstly, very-low-Ti (<1.5 wt.%) basalts are the most spatially abundant, and the surfaces with TiO$_2$ > 5 wt.% constitute less than 10% of the maria. Also, there occur two linear relationships between the FeO abundance (FA) and the TiO$_2$ abundance before and after the threshold, 16 wt.% of FA. Secondly, a new perspective about the mare volcanism is concluded with the volume FTAs in several important mare basins, although the conclusion should be severely treated with more sources of data. Thirdly, the FTAs in the lunar regolith change from depth to the uppermost surface, and the change is complex over the lunar surface. Finally, the distribution of the volume FTAs hints that the highlands crust is probably homogeneous at least in the microwave thermophysical parameters.

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1 INTRODUCTION

The FeO and TiO\textsubscript{2} abundances (FTAs) of the Moon are fundamentally significant to understand the origin and geological evolution of the Moon, so that the measurement of the FTAs on a global scale is always an important scientific objective for the current lunar exploration (Neal 2009; Wu 2012).

The FTAs are two compositions that show special spectral features in visible and near-infrared ranges, which makes them be accurately identified in remote sensing field (Neal 2009; Wu 2012; Wu et al. 2012). Currently, the FTAs have been successfully derived from the measurements in the visible-near-infrared wavelength range. The method developed by Lucey et al. (Lucey et al. 1998, 2000) is widely accepted to retrieve FTAs with Clementine UV-VIS data. Gillis et al. (Gillis et al. 2004) improved the Lucey’s method and developed a dual-regression method to better estimate the TiO\textsubscript{2} abundance inversion. Additionally, Shkuratov et al. (Shkuratov et al. 1999) mapped the FTAs of the lunar nearside using the Earth-based telescopic albedo data. Thereafter, data from the Kaguya Spectral Profile (SP) (Matsumaga et al. 2008), Chang’er-I Moon Mineralogy Mapper (M\textsuperscript{3}) (Pieters et al. 2009), and Chang’E Interference Imaging Spectrometer (IIM) (Wu 2012; Wu et al. 2012; Yan et al. 2012) were also extensively employed to map the FTAs of the Moon with a relatively better spatial or spectral resolution.

However, the inversion of the FTAs was doubted by Pieters et al. through analyzing the relationship between composition and reflectance spectrum of the lunar mare regolith (Pieters et al. 2008). This is also the reason that the retrieved FTAs are not widely used in lunar science (Pieters et al. 2008; Jiang and Jin 2011). Moreover, the inverted FTAs with optical data have poor penetration capabilities, which is only about few microns deep in the uppermost lunar regolith (Fa and Wieczorek 2012; Meng et al. 2014). Morgan et al. (Morgan et al. 2016) and Meng et al. (Meng et al. 2018a) have proved the great difference of the regolith compositions in depth to the superficial layer postulated by Hiesinger et al. (Hiesinger et al. 2000) in mare Imbrium. Thus, to better understand the geological features of the Moon, the volume FTAs with certain depth will be more interesting than those in the superficial layer indicated by the optical data.

To obtain FTAs within a certain depth of the lunar regolith, the Gamma-Ray Spectrometer (GRS) data from Lunar Prospector (LP) were used, and the penetration depth of the data could be up to several tens of centimeters (Lawrence et al. 1998; Elphic et al. 2000; Feldman et al. 2002; Prettyman et al. 2006). The results show apparently differences from the aforementioned retrievals. However, the spatial resolution of the GRS data is rather poor, which severely restricts the extensive applications of the inversed volume FTAs. Therefore, to get the FTAs of the lunar regolith to a certain depth with a proper spatial resolution is of essential importance to the current lunar study.

In Chinese lunar exploration project, a microwave sounder (CELSM) was aboard the Chang’E (CE) satellites with the purpose to measure the brightness temperature of the lunar regolith. The penetration depth of the CELMS data can be up to several meters (Wang et al. 2010; Jiang and Jin 2011; Meng et al. 2014; Pabari 2016), and the spatial resolution is better than that of LP-GRS data. Chan et al., Zheng et al., Meng et al., and Hu et al. have proved the strong correlation between the CELMS data and the FTAs based on the observations and the theoretical model using radiative transfer model (Chan et al. 2010; Zheng et al. 2012; Meng et al. 2016, 2018a; Hu et al. 2018). Therefore, the CELMS data provide a best candidate to evaluate the volume FTAs of the lunar regolith.
However, the CELMS data are hardly used to retrieve the volume FTAs of the lunar regolith directly with the theoretical model for the following reasons. Firstly, the theoretical model requires the critical lunar regolith parameters, including the temperature profile, dielectric constant, particle size, buried rocks and surface roughness. Unfortunately, the knowledge about such parameters is rarely sufficient (England et al. 1975; Keihm 1984; Jiang et al. 2008; Fa and Wieczorek 2012; Meng et al. 2014). Secondly, the inversion of FTAs with the theoretical model is related to the solution of non-linear integer-differential radiative transfer equations, which may likely lead to the ‘ill-posed’ problems (Keihm 1984; Fa and Wieczorek 2012; Meng et al. 2014). So how to avoid the influence from the aforementioned disadvantages of the theoretical model and to provide an efficient way to extract the volume FTAs of the lunar regolith still remains as a crucial problem in current lunar research.

As an excellent nonlinear fit theory, the back propagation neural network (BPNN) method has been widely used in the information extraction, target identification and biomedical engineering (Montopoli et al. 2011; Li et al. 2012; Meng et al. 2014). With the BPNN methodology, Meng et al., Li et al., and Montopoli et al. successfully evaluated the certain regolith parameters over the lunar surface (Montopoli et al. 2011; Li et al. 2012; Meng et al. 2014). This makes the BPNN method be an appealing candidate to estimate the FTAs of the lunar regolith. In this paper, the BPNN method is selected as an attempt to invert the volume FTAs of the lunar regolith using the CELMS data from CE-2 lunar orbiter. In Section 2, the architecture of the BPNN network and the training procedure are described. Additionally, the CELMS data and the Lunar Orbiter Laser Altimeter (LOLA) data are processed to obtain the brightness temperature ($T_B$) and the surface slope, respectively. Then the volume FTAs of the lunar regolith are retrieved using the BPNN method as shown in Section 3. The rationality of the inversed FTAs is also analyzed. Section 4 presents several important implications of the retrieved FTAs. The conclusions are showed in Section 5.

2 METHODOLOGY

2.1 BPNN Construction and Training

BPNN resembles the human brain in that the model learns and stores knowledge (Mehra and Wah 1992), which comprises several idealized layers of nodes and is specified by the weights, the learning rules, network interconnection geometry, and dimensionality. For BPNN takes nonlinearity into account using the sigmoid functions that connect the BPNN layers of nodes, the errors can be significantly decreased through the back propagation learning process.

The construction of the BPNN network has been thoroughly described in many literatures (Lippmann 1987; Rumelhart and McClelland 1987; Montopoli et al. 2011; Li et al. 2012; Meng et al. 2014). Considering the close correlation between the CELMS data and the volume FTAs, a one-hidden layer of nodes is applied in this study. Thus, a three-layer neural network algorithm is constructed: one input layer, one hidden layer, and one output layer (Figure 1). Note that the input, $X_{ij}$ (t = 1, 2, ..., T; j = 1, 2, ..., N), is the jth parameter of the tth sample, and N is the number of the specified parameters for every input sample; and the output, $O_{ts}$ (t = 1, 2, ..., T; s = 1, 2, ..., M), is the sth parameter of the corresponding tth sample, and M is the number of the given parameters for every output sample. T is the total sets of the available samples for network training.

According to the simulation results, the relationship between the $T_B$ and the volume FTAs is highly influenced by the surface slope $\theta$ (Fa and Wieczorek 2012; Meng et al. 2014, 2016; Hu et al. 2018). Onboard CE-2 lunar orbiter, the CELMS instrument operated at four channels. Therefore, the four-channel $T_B$ concluded from CE-2 CELMS data and $\theta$ estimated with LOLA data are selected as the input parameters to construct the BPNN network.

Therefore, to the input $X_{ij}$ (t = 1, 2, ..., T; j = 1, 2, ..., N), $T_B$ (i = 1, ..., 4) and $\theta$ are input parameters, and N is 5. The output $O_{ts}$ (t = 1, 2, ..., T; s = 1, 2, ..., M), the FTAs are set as
Table 1  Regolith parameters at Apollo (A), Luna (L) and Surveyor (S) landing sites (Shkuratov et al. 1999).

<table>
<thead>
<tr>
<th>location</th>
<th>Lat. (°)</th>
<th>Long. (°)</th>
<th>input parameters</th>
<th>output parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>3 GHz</td>
<td>7.8 GHz</td>
</tr>
<tr>
<td>A11(X1)</td>
<td>0.7N</td>
<td>24.3E</td>
<td>237.32</td>
<td>242.2</td>
</tr>
<tr>
<td>A12(X2)</td>
<td>3.2S</td>
<td>23.4W</td>
<td>234.56</td>
<td>240.23</td>
</tr>
<tr>
<td>A14(X3)</td>
<td>3.7S</td>
<td>17.5W</td>
<td>233.79</td>
<td>236.75</td>
</tr>
<tr>
<td>A15(X4)</td>
<td>26.1N</td>
<td>3.7E</td>
<td>228.54</td>
<td>223.35</td>
</tr>
<tr>
<td>A16(X5)</td>
<td>9.0S</td>
<td>15.5E</td>
<td>234.99</td>
<td>231.91</td>
</tr>
<tr>
<td>A17(X6)</td>
<td>20.2N</td>
<td>30.8E</td>
<td>232.41</td>
<td>228.86</td>
</tr>
<tr>
<td>L16(X7)</td>
<td>0.68S</td>
<td>56.30E</td>
<td>239.48</td>
<td>242.40</td>
</tr>
<tr>
<td>L20(X8)</td>
<td>3.57N</td>
<td>56.50E</td>
<td>240.36</td>
<td>233.64</td>
</tr>
<tr>
<td>L24(X9)</td>
<td>12.25N</td>
<td>62.20E</td>
<td>233.68</td>
<td>235.11</td>
</tr>
<tr>
<td>S5(X10)</td>
<td>1.41N</td>
<td>23.18E</td>
<td>238.10</td>
<td>244.37</td>
</tr>
<tr>
<td>S6(X11)</td>
<td>0.46N</td>
<td>1.37W</td>
<td>236.59</td>
<td>238.55</td>
</tr>
<tr>
<td>S7(X12)</td>
<td>41.01S</td>
<td>11.41W</td>
<td>212.54</td>
<td>208.16</td>
</tr>
</tbody>
</table>

note: the data in columns of 3.0 GHz, 7.8 GHz, 19.35 GHz, and 37 GHz are selected Tb at the noontime.

the output of the BPNN network and the dimension of the output layer M is 2. Moreover, due to the absences of the lunar regolith samples, only the regolith parameters at the Apollo, Luna and Surveyor landing sites are available to train the BPNN network. Thus, the total number of the available samples, T, is 12 (Table 1). Here, the used FTAs are measured during the Apollo (A), Luna (L), and Surveyor (S) missions, which are thought as the volume values.

Thereafter, the Generalized Delta Rule is used to train the three-layer BPNN network. The first layer distributes the input parameters selected from the previous analysis. The values of the nodes in the hidden layer are the summation of each input parameter multiplied by its connection’s weights to the corresponding nodes. Each node of the third layer receives the output from the node of the second layer, during which it is processed through a function and weighted again. The training process and weights are determined separately for each training pair using the sigmoid function, which enables the network to model the nonlinear problems (Li et al. 2012; Meng et al. 2014).

The goal of the training process is to optimize the weights for every node by minimizing the difference between the actual network output and the measurements. The BPNN changes the
Retrieving Volume FeO and TiO$_2$ Abundances of ...

Fig. 2 Scatter map of the CELMS data at noon in Copernicus crater (Meng et al. 2019).

weights of all nodes in the middle layer through the feedback process to minimize average error (E) of the system. When E reaches a minimum threshold, or the total number of iterations reaches a limited time, the training process of the BPNN is completed. Originally, 12 training pairs at Apollo, Luna and Surveyor landing sites are available to train the BPNN network. However, the amount of training examples is severely insufficient. To improve the BPNN training quality, the 12 training pairs are used ten times or more, which is equivalent to 120 or more training pairs available. Moreover, according to the training results, the number of the neuron at the hidden layer is set to 9, the predetermined threshold is set to $5\%$ of the average measurements, and the total number of iterations is set to 1000. Once trained, all the node weights are optimized and the BPNN model is ready for predicting the FTAs with the new input parameters, including four-channel $T_B$ data and the $\theta$.

2.2 CELMS Data Processing

CE-2 lunar orbiter was launched successfully on 1 October, 2010, and finished its observations on 9 June, 2011. The orbit altitude is about 100 km. The CELMS instrument is used to investigate the $T_B$ of the lunar regolith, which operates at 3.0, 7.8, 19.35 and 37.0 GHz. The observation angle is $0^\circ$ (Cai and Lan 2017; Meng et al. 2017). In this study, Level 2C swath data are used, which are the raw data processed after geometric correction and radiometric calibration. Their archive format is Planetary Data System (PDS). As a single file, the level 2C data contain a header and a table of measured data, which comprise the observation time, four-channel $T_B$s, solar incidence angle and azimuth angle, selenographic latitude and longitude, et al. (Fang and Fa 2014; Meng et al. 2016). According to the prelaunch calibration experiments, the radiometric accuracy is better than 1.0 K depending on temperature and frequency.

The nominal spatial resolution is 15 km for channels 7.8, 19.35 and 37.0 GHz, and is 25 km for 3.0 GHz (Cai and Lan 2017; Meng et al. 2019). But after overlying the obtained CELMS data on the lunar surface (Figure 2), $1^\circ$ spatial resolution along the latitude and very high spatial resolution along the longitude are clearly presented. Therefore, $1^\circ \times 1^\circ$ is a proper spatial resolution to generate the global $T_B$ maps, and the fitting scheme used is a seven-degree polynomial method. What’s more, through comparison of the CELMS data and the FTAs obtained with Clementine UV-VIS data, Chan et al. (Chan et al. 2010), Zheng et al. (Zheng et al. 2012), and Meng et al. (Meng et al. 2018a) presented that the $T_B$ at noon shows strong correlation with the FTAs. Therefore, only the $T_B$ at noon is employed in this study.
Noted that the value of $T_{Bi}$ ($i = 1, \ldots, 4$) ranges from 100 K to about 300 K, this is not acceptable to get a good result using the BPNN method with the sigmoid function (Elphic et al. 2000; Li et al. 2012). Therefore, the $T_B$ needs to be normalized, $nT_B$, with Eq. (1).

$$nT_{Bi} = (T_{Bi}(m, n) - \min(T_{Bi}(; n)))/\left(\max(T_{Bi}(; n)) - \min(T_{Bi}(; n))\right)$$  (1)

Where $(m, n)$ is the position of the study point, the range of $m$ is $(1, 2, \ldots, 360)$ and $n$ is $(1, 2, \ldots, 180)$. $i$ is $(1, 2, 3, 4)$, and $T_{Bi}$ represents one of the four-channel CELMS data. $T_{Bi}(; n)$ is the data series in the nth line. $\max(T_{Bi}(; n))$ is the maximum of the $T_{Bi}(; n)$, and $\min(T_{Bi}(; n))$ is the minimum one. Figure 3 is the $nT_B$ map at 37 GHz, whose range is reset as 0 to 1.

2.3 LOLA Data Processing

In macroscale, $\theta$ may alter the effective solar illumination of the lunar surface, which indirectly changes the microwave thermal emission of the lunar regolith (He et al. 2013; Meng et al. 2014; Hu et al. 2018). Therefore, according to the method provided by Rosenberg et al. (Rosenburg et al. 2011), the distribution of $\theta$ was estimated from the LOLA data of the LRO satellite. The LOLA data were acquired from 17 September 2009 to 9 March 2010, which were downloaded from http://pds-geosciences.wustl.edu/. Considering the spatial resolution of the $T_B$ maps, the mean $\theta$ in one CELMS pixel is employed as the new lunar surface parameter. Additionally, the $\theta$ range is from $0^\circ$ to about $25^\circ$, which is normalized with Eq. (2).

$$n\theta = (\theta(m, n) - \min(\theta(; n)))/\left(\max(\theta(; n)) - \min(\theta(; n))\right)$$  (2)

Where $n\theta$ is the normalized $\theta$, $\theta(; n)$ is the data series in the nth line. $\max(\theta(; n))$ is the maximum of the $\theta(; n)$, and $\min(\theta(; n))$ is the minimum one. Figure 4 is the $n\theta$ map, whose range is from 0 to 1.

Additionally, the azimuth of $\theta$ is also important in impacting the $T_B$ of the lunar regolith (Meng et al. 2014; Hu et al. 2018). There are two reasons for us to neglect the parameter. Firstly, the observation angle of the CELMS instrument is $0^\circ$, so that the influence of the azimuth is weaken to some extent. Secondly, the surface topography plays a weak role in the $T_B$ in middle and low latitude regions, which has been proved by the comparative studies in Hertzsprung basin and Mare Imbrium (Meng et al. 2018a,b).
3 FTAS RETRIEVAL

In this section, the volume FTAs of lunar regolith are retrieved and evaluated with those estimated with GRS data and UV-VIS data.

3.1 Retrieval of FTAs

Employing the trained BPNN network, to any given set of input parameters, the BPNN will rapidly generate a series of output values \( O = [O_1, O_2]^T \). Here, \( O_1 \) is the volume FeO abundance (FA), and \( O_2 \) is volume TiO\(_2\) abundance (TA). Through this way, the volume FTAs of the lunar regolith (Figure 5) can be efficiently retrieved using the generated \( nT_B \) and \( n\theta \) in the previous section.

Figure 5 shows that the retrieved FTAs in the maria are much higher than those in the highlands, and the inversed FA is apparently much higher than the TA, which agree with the current knowledge about the surface FTAs distribution of the Moon. Secondly, the FA in the maria varies widely from about 5 to 18 (wt.) and the TA changes from about 2 to 6 (wt.%), while the FTAs at the highlands are rather low, which is largely less than 5 wt.% of FA and 2 wt.% of TA. This is much lower than those estimated with the spectral and GRS data. Interestingly, Korokhin et al. (Korokhin et al. 2008) employed a non-linear analysis of Clementine UV-VIS data and LSCC data to prognosticate the TA in lunar soil and they concluded that the TA in highlands is less than 2%. Similar results were also suggested by Wu et al. (Wu et al. 2012) and Wu (Wu 2012) using the CE-1 IIM data. This coincides well with our results, hinting that the retrieved FTAs are rational and the BPNN method is feasible to evaluate FTAs with the CELMS data.

But two phenomena should be mentioned in Figure 4. Firstly, there are abundant belts in the northern hemisphere. This may be resulted from the used CELMS data, because the CELMS data could not cover the whole Moon surface at specific time and the data in the belts are fitted but not measured values (Chan et al. 2010; Zheng et al. 2012). Secondly, the retrieved FTAs are abnormally large in the high latitude regions. The main cause to such phenomenon might be that the sampled parameters are collected from Apollo, Luna and Surveyor landing sites, which are all in the low and middle latitude regions. Hence, the BPNN method is not suitable for the FTAs evaluation in the high latitude regions for the limitation of the sampling positions.
3.2 Rational Analysis

The validation of the retrieved parameters in remote sensing field is highly dependent on the “Ground Truth” Data. Until now, the FTAs are successfully evaluated with the Clementine UV-VIS data (Lucey et al. 1998, 2000; Gillis et al. 2004), CE IIM data (Wu 2012; Wu et al. 2012; Yan et al. 2012), and LP-GRS data (Lawrence et al. 1998; Prettyman et al. 2006). In this study, the FTAs evaluated with Clementine UV-VIS data (Figure 6) (Gillis et al. 2004) and LP-GRS data (Figure 7) (Prettyman et al. 2006) are employed as the “Ground Truth” to evaluate the inversed FTAs. Also, the FTAs inversed with CE IIM data are introduced for reference.
3.2.1 Comparison with Clementine FTAs

Generally, direct comparison between CELMS FTAs and Clementine FTAs gives a largely similarity. Firstly, very low FTAs exist in the highlands, while high FTAs occur in the mare and several large basins. Secondly, the relatively higher FA both occurs in mare Tranquillitatis, Fecunditatis, Humorum, Vaporum, Imbrium, and Oceanus Procellarum, while the high TA mainly exists in mare Tranquillitatis, Imbrium, and Oceanus Procellarum.

In local scale, Figures 5 and 6 both present that the relatively higher FTAs occur in the middle of Oceanus Procellarum, western part of mare Imbrium, southeastern part of mare Vaporum, and eastern part of mare Nubium. Also, the FTAs in the southern part of Orientale basin are higher than that in the northern. Particularly, the FTAs in Apollo basin (36.1°S, 151.8°W) are obviously higher than the nearby regions. And in mare Australe, the distribution of the regions with high FA of CELMS results is highly consistent with that of the Clementine results. Also, the Clementine FTAs and CELMS FTAs indicate a small patch with very low values surrounding Struve crater (23.0°N, 76.6°W), in the northwestern part of Oceanus Procellarum.

Therefore, our results are rational in local and global scales compared to the Clementine FTAs.

3.2.2 Comparison with LP-GRS Elemental Abundances

Figure 7 shows the FTAs maps determined by LP-GRS data (Prettyman et al. 2006). However, for the low spatial resolution of the GRS data, the detailed comparison between the LP-GRS results and the CELMS results can hardly be obtained. Besides the coincidence of the global distribution of the two results, they also postulate a good agreement in mare Imbrium and Oceanus Procellarum in regional scale.

Interestingly, in some mare areas, such as mare Serenitatis, Fecunditatis, Moscoviense, and Crisium, LP-GRS and CELMS TAs are similarly low. Especially in mare Crisium, LP-GRS TA

Fig. 7 Mapping of the FeO (a) and TiO\textsubscript{2} (b) abundances with LP-GRS data (Prettyman et al. 2006).
Retrieving Volume FeO and TiO$_2$ Abundances of ...

and CELMS TA both present very low values, which was supported by the measurement of the Luna 24 sample (Lawrence et al. 2002; Elphic et al. 2002). These distributions are apparently different from the Clementine results. Moreover, in mare Tranquillitatis, the CELMS FA agrees well with the Clementine and LP-GRS results, while the LP-GRS TA and CELMS TA are higher in the north basin floor than that in the south, different from Clementine TA. What’s more, the CELMS TA is nearly the same as that of the LP-GRS TA. The CELMS TA has a range of up to about 7 wt.%, and the LP-GRS TA in most extensive regions does not go above 8 wt.% (Lawrence et al. 2002), which are both apparently less than the Clementine TA.

Our results also show a good coincidence with the CE IIM results from Wu et al. (Wu et al. 2012) not only in the data range but also in the following typical regions. The first region is in mare Serenitatis and Tranquillitatis, where Clementine FA in the former is similar as that in the latter. But the CELMS and IIM FAs in mare Serenitatis are both much lower than that in mare Tranquillitatis. The second region is in mare Moscoviense and Orientale, CELMS and IIM results both indicate a considerably high FA value as that in the western part of mare Imbrium, while Clementine results show a rather low FA value.

Generally, the retrieved FTAs are fairly close to that obtained with the three datasets in the spatial distributions and they coincide well with LP-GRS and CE-IIM FTAs in values. The comparison not only validates that the estimated FTAs with the CELMS data are rational, but also hints the difference of the four results in understanding the lunar geological features.

4 GEOLOGICAL SIGNIFICANCES

The global maps of FA and TA derived from CELMS data enable us to re-evaluate the statistical characteristics of FeO and TiO$_2$, their relationship across the Moon, and the geological features of the lunar surface.

4.1 New Views about FTAs Distributions

The statistical analysis shows that the surfaces with TA $>$ 5 wt.% constitute less than 10% of the maria, while very-low-Ti (<1.5%) basalts are the most spatially abundant and high-Ti basalts are the least. This is considerable to the LP-GRS and CE IIM results, but it is much different from the Clementine results. Lucey et al. (Lucey et al. 2000) found that the maria surfaces with TA $>$ 5 wt.% constitute only 20% of the maria. Moreover, the TA derived by Giguere et al. (Lucey et al. 2000) and Wu et al. (Wu et al. 2012) shows that the far side maria is dominated by very-low-Ti basalts, but the CELMS results indicate a relatively higher TA in the far side, particularly in mare Moscoviense and the southwestern part of Apollo basin.

Figure 8 shows the histograms of the FTAs for the entire CELMS data set, which present several aspects different from the previous results (Lucey et al. 2000; Prettyman et al. 2006; Wu et al. 2012). The first aspect is the shapes of the the FA and TA histograms. The histogram of FA has three peaks, where the first and second highest peaks are both corresponding to mare and the lowest one is related to the highlands. The histogram of the TA is a unimodal continuum distribution. Secondly, the lowest modal FA of about 2.26 wt.% is apparently lower than the Clementine modal abundance given by Lucey et al. (Lucey et al. 1998) and Gillis et al. (Gillis et al. 2004). Interestingly, the highest modal FA is close to the average LP-GRS abundance given by Prettyman et al. (Prettyman et al. 2006) and the M$^3$ abundance provided by Zhang and Bowles (Zhang and Bowles 2013). Moreover, the modal TA indicated by the histogram is much lower than that given by Lucey et al. (Lucey et al. 2000), while it is similar with the IIM modal abundance given by Wu et al. and Wu if the largest and lowest modals are omitted, which are mainly caused by the topography (Wu et al. 2012; Wu 2012). Similarly as FA modal, the highest average TA determined in this study is found in mare Tranquillitatis, about 4.03 wt.%, which is comparable to the results determined by Zhang and Bowles (Zhang and Bowles 2013) and Korokhin et al. (Korokhin et al. 2008).
The data from the lunar samples show that TA shows a complex relationship with FA in mare basalt (Heiken et al. 1991; Wu et al. 2012). With the FTAs estimated with IIM data, Wu et al. thought that the relationship between FA and TA exhibits a slightly obtuse-triangle field covering a space similar to the returned samples (Wu et al. 2012). Figure 9 shows the scatterplots of FA and TA estimated with the CELMS data, which indicates a steep, well-defined increase with FA for the regions with the high TA. Two features of Figure 8 should be noticed. Firstly, although the relationship between FA and TA is nonlinear, this correlation is apparently better than that indicated by the optical results. Secondly, the relationships between FA and TA are obviously linear before and after the threshold, about 16 wt.% of FA. The two linear relationships may hint a different view about the mare volcanism over the lunar surface.

4.2 A New View about Mare Volcanism

What we know about the mare volcanism is mainly from the distribution of the FTAs over the lunar surface. Compared to the optical results, Figure 5 indicates a new view about the mare volcanism represented by the following several regions.
Firstly, in Oceanus Procellarum, Figure 5 shows that the regions with high FTAs mainly exist in the middle part along the latitude and they extend as a broad belt region from the north to the south. Interestingly, this distribution can be partly supported by the Clementine TA distribution in Figure 6(b). Additionally, the optical results indicate that the belt region is not continuous, while the CELMS FTAs indicate a continuous belt region with high values. The difference between the Clementine results and the CELMS results is probably from the contamination of the impact ejecta from other regions, which plays an important role in the measured optical data (Lucey et al. 1998; Wu et al. 2012). After all, Aristarchus, Copernicus and Kepler craters are located not far from the belt, and even the ejecta from Tycho crater in far distance also altered the surface compositions to some extent (Desai et al. 2014). Moreover, Head et al. and Haruyama et al. suggested that the higher-FTAs basalts mostly appear in the younger basalts (Head et al. 1978; Haruyama and Josset 2009). Considering the relationship between the age and the FTAs, such phenomenon implies the existence of the last stage of mare basalts in Oceanus Procellarum, which also gives some clues to look for the sources of the mare basalts.

Secondly, in mare Crisium, Figure 5 postulates a different view compared to the Clementine FTAs. Figure 6(a) shows that most portion of Crisium basin is filled with high-FA basalt, while Figure 6(b) presents high TA values in the southeastern basin floor. That is, the agreement between the FA and TA in the basin is not good. Considering the abundant large craters as Peirce and Picard inside the basin and Proclus and Eimmart surrounding the basin, it is likely the crater ejecta that changes the surface compositions of the lunar regolith. This is also the cause that, though Head et al. (Head et al. 1978), Sliz and Spudis (Sliz and Spudis 2016), and Spudis and Sliz (Spudis and Sliz 2017) gave their understanding about the geological units in mare Crisium, the interpreted results are greatly different from each other.

Compared to the optical results in Figure 6, Figure 5 presents that the highest FTAs only exist in the most eastern portion of the basin floor, Alhazan unit. Moreover, the FTAs in the other portion of the basin floor are similar, which are higher than the nearby highlands but apparently lower than those in Alhazan unit. This indicates that the mare basalts in the Crisium basin should only be divided into two stages, much different from the previous results (Head et al. 1978; Sliz and Spudis 2016; Spudis and Sliz 2017). Furthermore, Head et al. (Head et al. 1978) and Haruyama et al. (Haruyama and Josset 2009) suggested that the higher-FTAs basalts mostly appear in the younger basalts. Thus, the distribution features of the FTAs postulate that the last stage of mare basalt should exist in Alhazan unit and this is also the origination area of the lava for the whole Crisium basin. Thereafter, the late impact events strongly alter the superficial layer of the mare basalts. Similar conclusion is also obtained by directly analyzing the microwave thermal emission of the mare basalts using the CE-2 CELMS data and the LRO WAC data (Meng et al. 2018c).

Thirdly, the retrieved FTAs in mare Serentatis are also rather different from the Clementine results. Figure 6 indicates that the FA in mare Serentatis is largely similar as that in mare Tranquillitatis, while the TA in the former is much less than the latter. But the CELMS results in Figure 5 shows that both the FA and the TA in mare Serentatis are much less than those in mare Tranquillitatis, especially the FA. Combined with the penetration features of the two datasets, this indicates that the high FA only exists in the superficial layer of mare Serentatis, and that the FTAs in depth layer penetrated by the CELMS data are low. Also, the LP-GRS FTAs present low values in the mare, validating the rationality of our results. Additionally, the FTAs values are lower than those in the eastern part of mare Imbrium and they are nearly similarly low as those in the north highlands. Therefore, the mare volcanism derived with the Clementine FTAs should be severely treated with more sources of data in this field.

Last but most importantly, Giguere et al. (Giguere et al. 2000) shows that the maria in the lunar farside is dominated by very-low-Ti basalts according to Clementine results. However, Figure 5 indicates that the FTAs in several important regions such as mare Moscoviense, Apollo basin, and Tsioïkovskiy crater are much higher than those in the Clementine results. Moreover,
the FTAs in the three mentioned regions are similarly high as those in the middle of Oceanus Procellarum and western part of Mare Imbrium, indicating a relatively younger mare basalts in the lunar farside as those in the nearside. Such conclusion can also be verified by the findings of Head et al., Haruyama et al., and Pasckert et al. (Head et al. 1978; Haruyama and Josset 2009; Pasckert et al. 2018), who suggested the existence of the young mare basalts in the lunar farside with the crater size-frequency distribution method. Therefore the mare volcanism in the lunar farside should be re-acknowledged with more sources of data in future. We also hope that these findings would be helpful to better use the in-situ data measured by the CE-4 YUTU-2 rover.

4.3 Changing of FTAs with Depth

The previous discussions indicate that the retrieved FTAs with CELMS are acceptable. Meanwhile, the FTAs estimated with Clementine UV-VIS (Gillis et al. 2004) and with LP-GRS data (Prettyman et al. 2006) are widely accepted in current Moon research (Korokhin et al. 2008; Wu et al. 2012; Zhang and Bowles 2013). Considering the penetration depth of the UV-VIS signal, GRS signal and CELMS signal, Figure 6, Figure 7 and Figure 5 probably hint the change of FTAs with depth in the lunar regolith.

The penetration depth of the UV-VIS signal is only several microns, the penetration depth of the GRS signal is up to 50 cm, and the CELMS signal can penetrate the lunar regolith up to several meters (Jin et al. 2003; Fa and Wieczorek 2012). That is, Figure 6 indicates the FTAs of the uppermost lunar regolith, Figure 7 presents the FTAs in several tens centimeters of the lunar regolith, while Figure 5 is largely the average FTAs in the several meters of the lunar regolith. The comparison of Figure 6, Figure 7 and Figure 5 represents the change of the FTAs from the uppermost layer to certain depth in lunar regolith. Figure 6 hints that the FTAs are largely high in Oceanus Procellarum, especially in the middle and southwestern part. Whereas, Figure 7 indicates that the area with high FTAs is much less than those at Figure 6. Interestingly, Figure 5 presents that only the middle of Oceanus Procellarum has the high FTAs, which is largely similar to that in Figure 7. Moreover, in mare Imbrium, the FTAs in the western part are a bit higher than those in the eastern in Figure 6, while Figure 7 and Figure 5 both postulate that the FTAs in the western part are much higher than those in the eastern. Also, in mare Serenitatis, only Figure 6 shows that the FA is high here, whereas Figure 7 and Figure 5 present that FA is rather low here. The aforementioned comparison indicates that the FTAs in the uppermost layer to some depth are different from that in the uppermost surface.

Figure 10 is the FA (a) and TA (b) estimated with CELMS data (Curve 1, line in blue color), LP-GRS data (Curve 2, line in green color) and Clementine UV-VIS data (Curve 3, line in red color), respectively, which represent the average FTAs in the depth layer, upper layer, and the uppermost layer of the lunar regolith. Figure 10 hints that the change of FTAs with depth is complex. Generally, the FTAs values estimated with UV-VIS data are the highest and those estimated with CELMS data are the lowest among the three kinds of dataset. That is, the FTAs are decreasing with depth. But, the FA in Sinus Aestrum (about 20°W to 5°W), Sinus Medii (about 5°W to 0°E), mare Fecunditatis (about 44°E to 60°E), and mare Smythii (about 80°E to 100°E) seemingly doesn’t vary with depth, which hints the homogeneity of the lunar regolith in these places. From such viewpoint, the similar distribution features of FTAs in mare Tranquillitatis, Nectaris and Humorum in Figures 5, 6, and 7 reveal that the lunar regolith is homogeneous there. Whereas, in mare Tranquillitais (about 19°E to 32°E), the FA is increasing with depth hinted by the three datasets. Such phenomenon not only implies the complexity of the lunar regolith in vertical direction, but also provides a new content which is worth to be further studied in future.
Retrieving Volume FeO and TiO$_2$ Abundances of ...

Fig. 10  Distribution of FeO (a) and TiO$_2$ (b) abundances along Moon Equator. Curve 1: Estimated with CELMS data; Curve 2: Estimated with LP-GRS data; Curve 3: Estimated with Clementine UV-VIS data.

4.4 Homogeneity of Lunar Highlands Crust

Pieters (Pieters 1993) and Tompkins and Pieters (Tompkins and Pieters 1999) found that the lunar highlands crust below the surface is compositionally diverse by investigating the mineralogy of the central peaks, representing materials from 5 to 30 km depth. Wu et al. (Wu et al. 2012) studied the elemental abundance trends of the topmost surface of the lunar highlands using the high resolution FA and TA maps estimated with IIM data and concluded that the lunar highlands crust is relatively uniform on the quadrant scale but inhomogeneous on the global scale.

However, as mentioned above, the optical spectrum is strongly affected by the impact ejecta, topography and other factors (Pieters 1999; Wu et al. 2012). That is, the conclusion from IIM data and UV-VIS data that the lunar highlands crust is inhomogeneous should be retreated. Figure 5 presents a distinctly different viewpoint about the compositional structure of the highlands crust in the following several aspects. Firstly, nearly the whole lunar highlands are indicated by considerably low volume FTAs. This conclusion is also verified in part by the TA estimated by Korokhin et al. (Korokhin et al. 2008) with Clementine data and by Wu with CE-1 IIM data (Wu 2012), and the FTAs estimated by Prettyman et al. (Prettyman et al. 2006) with LP-GRS data and by Zhang and Bowles (Zhang and Bowles 2013) with M$^3$ data, which show that the low values are uniformly distributed on almost the whole highlands. Secondly, in the south pole-Aitken (SPA) basin, the largest crater of the Moon, Figure 6 postulates that the Clementine FTAs in the whole basin are apparently higher than the surrounding highlands, while Figures 5 and 7 indicate that the relatively higher volume FTAs only occur in several small patches, but not the whole basin. Additionally, the volume FTAs in considerable regions are nearly similarly low as those in highlands regions, especially in the west part of Apollo basin and the western portion of the SPA basin. Thirdly, the FTAs around the typical large highlands craters are similar. Particularly in Hertzsrup basin (2°N, 128°W) with a diameter of 570 km, it excavated the lunar crust as deep as 40 km below the surface (Meng et al. 2018b). There does not occur FTAs changes from the basin center to far distance. Thus, the shallow lunar highlands crust is likely homogeneous at least in microwave thermophysical parameters.

What gets us in trouble is the the FA between mare Imbrium and mare Frigoris, which is much higher than that in other highlands places in Figure 5. This phenomenon is also pointed out by Wu et al. using both the M$^3$ and CE IIM data (Wu et al. 2018). This means that the high FA values in the region are not only on the surface layer, but also in depth layer.
Also, considering the ubiquitous low-calcium pyroxene and large amounts of olivine surrounding Imbrium distribution, Wu et al. speculated the change of the composition with depth in the lunar crust (Wu et al. 2018). This makes our conclusion about the homogeneity of the highlands crust in doubt. Even though, the CELMS FTAs postulate a different view about the compositions distribution of the shallow lunar crust compared to the visible results.

5 CONCLUSIONS

In the lunar mare volcanism study, the volume FTAs of the lunar regolith are more meaningful compared to the optical results. The measured CELMS data provides a potential way to evaluate the volume regolith FTAs of the lunar surface.

In this study, new global maps of the volume FTAs are derived with the CELMS data from CE-2 satellite. Firstly, the three-layer BPNN technique is constructed to retrieve the FTAs of the lunar regolith. With the TB data generated with the CELMS data, surface slope estimated from LOLA data and the corresponding FTAs obtained during the Apollo, Luna and Surveyor missions, the volume FTAs of the lunar regolith are retrieved with the BPNN method. Comparisons of the inverted volume FTAs to those estimated with Clementine UV-VIS data and LP-GRS data postulate that the volume FTAs are rational, which provides a new understanding about the elements about the Moon.

Firstly, the statistical analysis shows that the surfaces with TA > 5 wt.% constitute less than 10% of the maria, while very-low-Ti (<1.5%) basalts are the most spatially abundant and high-Ti basalts are the least. This is considerable to the LP-GRS results, but it is much different from the Clementine results. Also, the scatterplots of the volume FA and TA indicate that the relationships between FA and TA are obviously linear before and after the threshold, 16 wt.% of FA.

Secondly, the volume FTAs in mare Serenitatis, Crisium, Moscoviense, Oceanus Procellarum, and Apollo basin present a new view about the mare volcanism over the lunar surface. This is useful not only to pursuit the source of the mare basalts, but also to better understand the volcanic procedures in the important mare. The conclusion deserves to be further studied with more sources of data and even the in-situ measurements by YUTU-2 rover in the current CE-4 mission.

Thirdly, the comparisons between the CELMS, UV-VIS, and LP-GRS FTAs postulate that the FTAs in the lunar regolith to some depth are different from those in the superficial layer. The results hint the change of the FTAs with depth and the complexity of the lunar regolith in vertical direction.

At last, the low volume FTAs are widely distribution in almost the whole lunar highlands and in most patches of the SPA basin, which hints that the lunar highlands crust is likely to be homogeneous at least in the microwave thermophysical parameters.

Due to the limited number of samples and their spatial distribution, the inverted FTAs are not reliable at high latitude regions. With the further exploration of the moon, there will be more and more available input-output pairs for the BPNN network to improve the retrieval results. Also, several special features revealed by the volume FTAs are important to better understand the mare volcanism and the mineral distributions of the Moon, which deserves to be further studied with more sources of data and even the in-situ exploration.

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