A SPECTRAL TRANSFORMATION APPROACH FOR LASER-INDUCE BREAKDOWM SPECTROSCOPY (LIBS) QUANTITATIVE ANALYSIS. Guobin Jin[1], Zhongchen Wu[1, *], Changqing Liu[1], Zongcheng ling[1], Li Zhang[2]. [1]Shandong Provincial Key Laboratory of Optical Astronomy and Solar-Terrestrial Environment, Institute of Space Sciences, Shandong University, Weihai, Shandong, 264209, China (z.c.wu@sdu.edu.cn); [2]School of Mechanical, Electrical and Information Engineering, Shandong University, Weihai 264209, China.

Introduction: Zhurong rover of China's first Mars mission landed on the southern of Mars Utopia Planets successfully on May 15, 2021. Laser-Induce Breakdown Spectroscopy (LIBS) was adopted by the Mars Surface Composition Detector (MarSCoDe) on Zhurong rover for *in-situ* Mars exploration [1]. LIBS is a remote sensing technology to quickly obtain multi-element compositions of targets at a sub-millimeter scale which has already been applied on the exploration of the red planet (ChemCam and SuperCam) and obtained a large set of data to increase the human knowledge of Mars [1, 2, 3].

Partial Least Squares (PLS) is a classical chemometric method by constructing a linear multivariate regression model for spectral quantitative analysis [4]. It has been successfully applied to build several accurate prediction models for element analysis of ChemCam LIBS data such as SiO_2, TiO_2, Al_2O_3, FeO_T, MgO, CaO, Na_2O, K_2O [5, 6].

Herein, a spectral transformation approach was proposed to transform the LIBS spectra between two different LIBS system (i.e. ChemCam and SDU-LIBS [7]) whose data were partly different in characteristics. Based on this approach, SDU-LIBS spectra data were transformed into ChemCam uniform and then the two kinds of LIBS system can have more similar spectral features and can share one quantitative analysis model. This transformation is very useful for model cross validation of two kinds of different LIBS system, especially for planetary exploration.

Data and Methods: The SDU-LIBS data set used in this study was described in previous work [7]. As shown in Table 1, 11 samples of SDU-LIBS sample set were specially designed to be identical to ChemCam calibration samples which were used to test method applicability of our approach. In this work, the ChemCam calibration database [6] was used to build the PLS prediction model. The transformed SDU-LIBS data was used as test data set. Spectral pretreatments (such as noise removal and continuum removal) and band selection of SDU-LIBS were performed for getting better prediction results.

As shown in Figure 1, the framework diagram of our approach consists of 4 steps: Intensity Transformation, Wavelength Recalibration, Interpolation and Energy density Correction.

a. **Intensity Transformation** unified the intensity unit of two kinds of LIBS data sets.

b. **Wavelength Recalibration** calibrated the wavelength and pixel position of SUD-LIBS data set using ChemCam data as the standard.

c. **Interpolation** correction partly eliminates the differences of spectral step size and spectral profiles between two kinds of LIBS data.

d. **Energy density Correction** was used to eliminate the variation of laser excitation power.

Table 1. SDU-LIBS sample set.

No.	Sample Name	Reference ID	Rock Type
01	Andesite	AGV2	Igneous
02	Basalt	BHVO2	Igneous
03	Basalt	BIR1	Igneous
04	Andesite	GBW07104	Igneous
05	Basalt	GBW07105	Igneous
06	Limestone	GBW07108	Sedimentary
07	Gypsum	GYPD	Sedimentary
08	Andesite	JA2	Igneous
09	Andesite	JA3	Igneous
10	Basalt (Olivine)	MO14	Igneous
11	Sediments/shale (kerogen, carbonate)	SGR1	Sedimentary

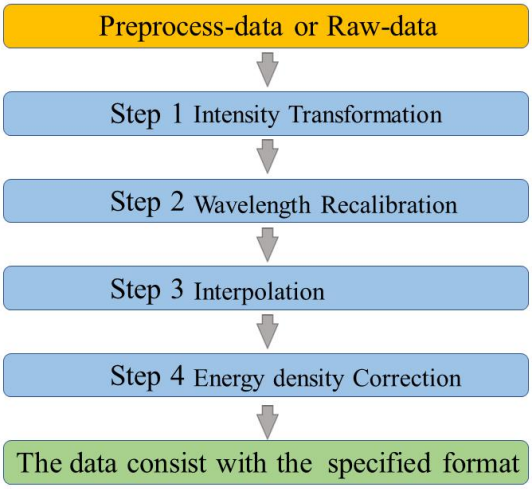

Figure 1. Framework Diagram of the data transformation approach.

The ChemCam calibration database was used to build the PLS prediction model. After 4 steps data correction, some spectral data of SDU-LIBS data were selected as test data to verify method applicability of our approach. Z-score normalization applied on each spectrum before building models.

Results: The relative intensity was changed after the Intensity Transformation. Some changes in peak profiles were also noticed after Interpolation step. RMSE (Root Mean Square Error) was used to describe this change which was calculated by using ten normalized peaks to O (emission line in 777 nm). The average RMSE of intensity and spectral profiles was 0.0121 and 0.0652 which indicated a very small changes after interpolation. After Energy density Correction, all the spectra who have been processed by the approach will be predicted by PLS model trained by ChemCam calibration database. The result of our approach only partly promoted the capability of two kinds of different LIBS data. The RMSEC (Root Mean Square Error of Calibration) of model and the RMSEP (Root Mean Square Error of Prediction) of SDU-LIBS after processed by our approach are listed in Table 2. All the elemental predictions (SiO_2, TiO_2, FeO_T, MgO, CaO, Na_2O, Al_2O_3, K_2O) are similar as their reference values. This indicated our spectral transformation approach is useful for model cross validation of two kinds of different LIBS system.

Table 2. The RMSEC and RMSEP (wt.%) of SDU-LIBS after the approach.

	RMSEC	RMSEP
SiO_2	4.8	12.3
TiO_2	0.5	1.0
Al_2O_3	3.2	6.2
FeO_T	3.2	2.1
MgO	1.7	10.0
CaO	2.2	8.8
Na_2O	0.8	1.1
K_2O	0.8	5.8

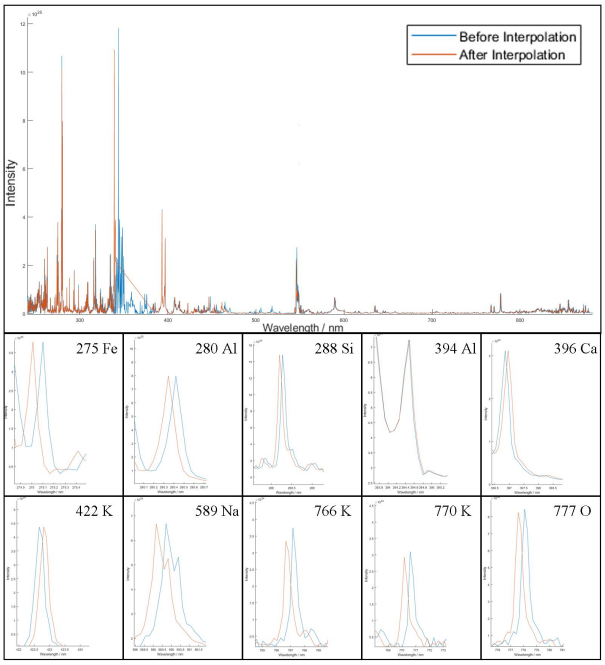

Figure 2. SDU-LIBS spectra before and after interpolation (Sample No.1).

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