Improving the spectral measurement accuracy based on temperature distribution and spectra-temperature relationship

Zhe Li, Jinchao Feng, Pengyu Liu, Zhonghua Sun, Gang Li, Kebin Jia

PII: S1350-4495(17)30800-9
DOI: https://doi.org/10.1016/j.infrared.2018.02.007
Reference: INFPHY 2498

To appear in: *Infrared Physics & Technology*

Received Date: 3 December 2017
Revised Date: 12 January 2018
Accepted Date: 15 February 2018

Please cite this article as: Z. Li, J. Feng, P. Liu, Z. Sun, G. Li, K. Jia, Improving the spectral measurement accuracy based on temperature distribution and spectra-temperature relationship, *Infrared Physics & Technology* (2018), doi: https://doi.org/10.1016/j.infrared.2018.02.007

Improving the spectral measurement accuracy based on temperature distribution and spectra-temperature relationship

Zhe Li[1,2,3,4], Jinchao Feng[1,2,3,4,*], Pengyu Liu[1,2,3,4], Zhonghua Sun[1,2,3,4], Gang Li[5] and Kebin Jia[1,2,3,4]

1. Faculty of Information Technology, Beijing University of Technology, Beijing, 100124, China

2. Beijing Laboratory of Advanced Information Networks, Beijing, 100124, China

3. Beijing Advanced Innovation Center for Future Internet Technology, Beijing University of Technology, Beijing, 100124, China

4. Beijing Key Laboratory of Computational Intelligence and Intelligent System, Beijing University of Technology, Beijing, 100124, China

5. College of Precision Instrument and Opto-Electronics Engineering, Tianjin University, Tianjin 300072, China

* Corresponding author: fengjc@bjut.edu.cn

Abstract Temperature is usually considered as a fluctuation in near-infrared spectral measurement. Chemometric methods were extensively studied to correct the effect of temperature variations. However, temperature can be considered as a constructive parameter that provides detailed chemical information when systematically changed during the measurement. Our group has researched the relationship between temperature-induced spectral variation (TSVC) and normalized squared temperature. In this study, we focused on the influence of temperature distribution in calibration set. Multi-temperature calibration set selection (MTCS) method was proposed to improve the prediction accuracy by considering the temperature distribution of calibration samples. Furthermore, double-temperature calibration set selection (DTCS) method was proposed based on MTCS method and the relationship between TSVC and normalized squared temperature. We compare the prediction performance of PLS models based on random sampling method and proposed methods. The results from experimental studies showed that the prediction performance was improved by using proposed methods. Therefore, MTCS method and DTCS method will be the alternative methods to improve prediction accuracy in near-infrared spectral measurement.

Keywords: Temperature-induced spectral variation; Calibration set selection; Temperature distribution;