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Consistency analysis of plastic samples based on similarity calculation from limited range of the Raman spectra

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Abstract. We proposed a novel method to calculate the similarity between samples with only small differences at unknown and specific positions in their Raman spectra, using a moving interval window scanning across the whole Raman spectra. Two ABS plastic samples, one with and the other without flame retardant, were tested in the experiment. Unlike the traditional method in which the similarity is calculated based on the whole spectrum, we do the calculation by using a window to cut out a certain segment from Raman spectra, each at a time as the window moves across the entire spectrum range. By our method, a curve of similarity versus wave number is obtained. And the curve shows a large change where the partial spectra of the two samples is different. Thus, the new similarity calculation method identifies samples with tiny difference in their Raman spectra better.

1. Introduction

The plastic safety parts are the critical parts of electrical products and have significant influence on the safety of electrical products. According to some regulations, China Compulsory Certification (CCC) for example, the plastic parts (non-metallic parts) of household electrical appliances or electrical products with similar applications are the critical part of safety. Moreover, the regulations required that all the materials and components of plastic parts for the productions be certified to be consistent with those of the test samples for type tests and declaration. Any changes to the materials or components of the plastic safety parts may affect the safety of electrical products. So the test of the consistency of the plastic safety parts is of great significance.

Chemical method is one of the most common methods for the consistency test of two plastic material samples. However, chemical method is of high cost and damages test samples. Raman spectrum detection method which uses Raman spectroscopy to detect the surface of samples and distinguish samples via spectrum analysis [1-2], has been widely study for its advantages of simplicity, convenience and high accuracy, and causing no damage to the samples [3].

To analyse the Raman spectrum data, one common approach is to extract the characteristic peaks and compare them with those of the standard samples in the standard database. It requires lots of work in building and improving the database. The other approach is to make similarity analysis of spectra between different samples [4]. It can distinguish samples with different materials more quickly and efficiently. However, this approach will be ineffective in distinguishing samples with same materials with different additives, such as additive type -- flame retardant in plastics. This is because the additive caused differences at only specific positions in Raman spectrum, but the similarity is calculated throughout the whole Raman spectrum range [5]. A simple but effective way to solve the problem is to calculate the similarity at a specific segment where the difference of the Raman spectrum of different samples appears. Nevertheless, it requires that we know the position of the calculation segment in the range [6].

Problems mentioned above are summarized as: 1) positions where differences appear in Raman spectra of different samples are unknown, and 2) the similarity calculated based on the whole range of Raman spectrum cannot distinguish samples with same materials but different additives. This paper proposed a novel spectrum analysis method named “moving window similarity calculation method.” The method uses a window with certain width scanning across the entire Raman spectra to calculate the similarity between the spectra of different samples in the window. Then a curve of similarity versus wave number is obtained. Therefore, the curve will have a large fluctuation where the Raman spectra of the two samples are quite different. To prove the validity of our methods, the Raman spectra of two ABS samples, one not added with flame retardant (Sample A), and the other added with flame retardant (Sample B) are tested and analysed. The experimental results show that the moving window similarity analysis method is an effective method for distinguishing samples with same materials but different additives.

2. Experimental

2.1. Experimental equipment
Xplora ONETM Raman microscope (France HORIBA Scientific) has the advantages of non-destructive analysis, high spatial resolution and high sensitivity [7]. Software such asLabSpecAppllication and Matlab were used to process and analyse the spectra.

2.2. Experimental samples
All the starting materials were commercially available and were used without further publication. ABS samples were supplied by Defenghang Company (Xiamen, China).

2.3. Experimental procedure
The samples were put on the platform of the Raman microscope. Then the focal length was adjusted to set the focus onto the surface of the samples. The excitation wavelength is 785nm, the spectral sampling interval is 1.02cm^{-1}, the spectral scanning range is 200-2000cm^{-1}, the integral time is 10s, the aperture of the optical path is 300mm and the slit of the spectrometer is 100mm. In this experiment, we randomly chose three positions of the both samples for testing and obtained six groups of Raman spectrum data.

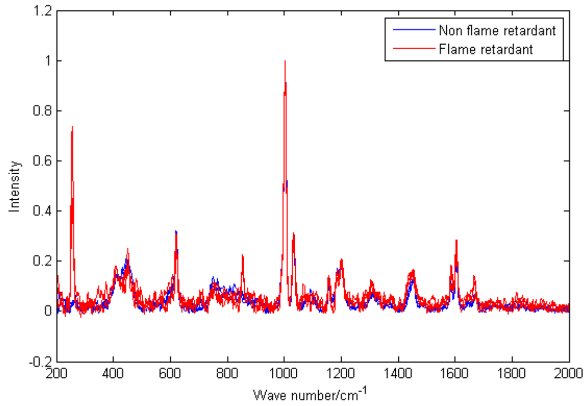

Figure 1. Spectrogram after preprocessing.

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After testing, the software LabSpecAppllication was used to preprocess the data. The preprocessing procedure was divided into three steps: smoothing filtering, fluorescent background subtraction, and normalization. The spectra after preprocessing are shown in Figure 1. It can be seen from Figure 1 that the spectra of two samples show a good reproducibility, respectively. The spectra of the two samples are similar in most positions except on the wave length near 250cm^{-1} where the flame retardant ABS sample has an obvious peak and the non-flame retardant sample has not.

3. Results and analysis

3.1. Similarity calculation

Each group of collected data consists of two vectors. The first vector is the discrete intervals of wave numbers (200-2000cm^{-1}). The second vector $\boldsymbol{X}$ is the normalized intensities corresponding to each wave number. Since the first vector of each group is the same, $\boldsymbol{X}$ is only needed to be used in calculating the similarity.

The method of calculating similarity is to use similarity function. In this paper we use the following generalized Jaccard coefficient function [8]:

$$sim(X_1, X_2) = \frac{X_1^T \cdot X_2}{\| X_1 \|^2 + \| X_2 \|^2 - X_1^T \cdot X_2} \tag{1}$$

This function can better amplify the difference between vectors as compared to other similarity functions [9]. The value of this function is from 0 to 1. The higher the value is, the greater the similarity of the two sample show. The similarity computed by this function is 0.9268, which cannot explain the inconsistency of the two samples.

3.2. Moving window method

The moving window method uses a certain width of window to scan across the entire spectrum and calculate the similarity of the spectra in the window while scanning. From equation (1) we can see that when both $\boldsymbol{X_1}$ and $\boldsymbol{X_2}$ are close to 0, minor fluctuations will result in a significant difference in the degree of similarity. So before using this method, the data were transformed as follows:

$$x_i' = 1.2 - x_i \tag{2}$$

In the above equation, as x_i is the element of $\boldsymbol{X}$, the value of x_i' is between 0.2 and 1.2, which can avoid the situation mentioned above. Since the test result gives a good reproducibility, we use the first groups of data of each sample for calculation. The window width is set to be 5 cm^{-1}, the central wave length of the window range between 205cm^{-1} and 1995cm^{-1}. The spectra and calculation results are shown is Figure 2.

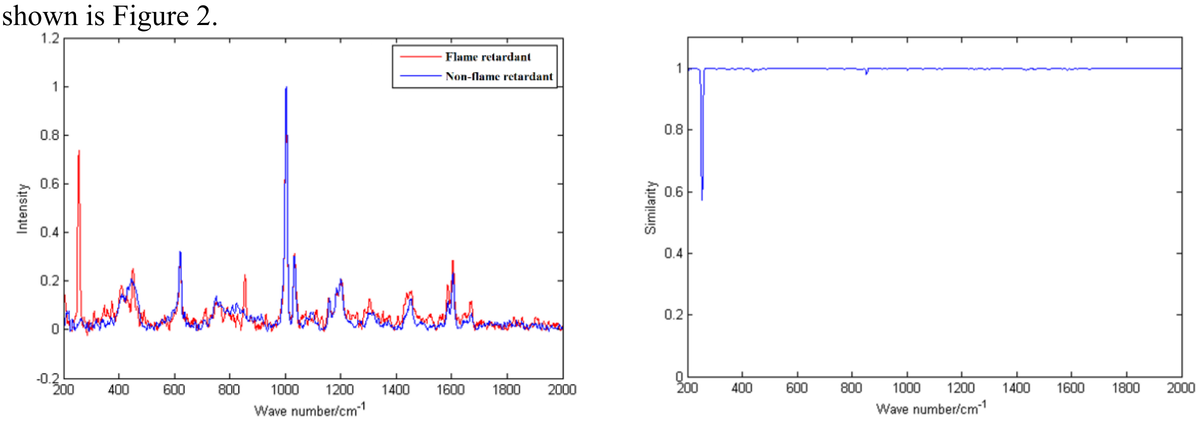

Figure 2. (a)Comparison of ABS samples' spectra with and without addition of flame retardant. (b) The results obtained by moving window similarity calculation method.

Figure 2 shows that, when the window moves to the peak which represents the flame retardant, the similarities decrease significantly, and that in other positions the similarities remain close to 1. In that case we can conclude that the two spectra belong to different samples. For comparison, we apply this method to two different test data of the same sample (without retardant), the results are shown in Figure 3.

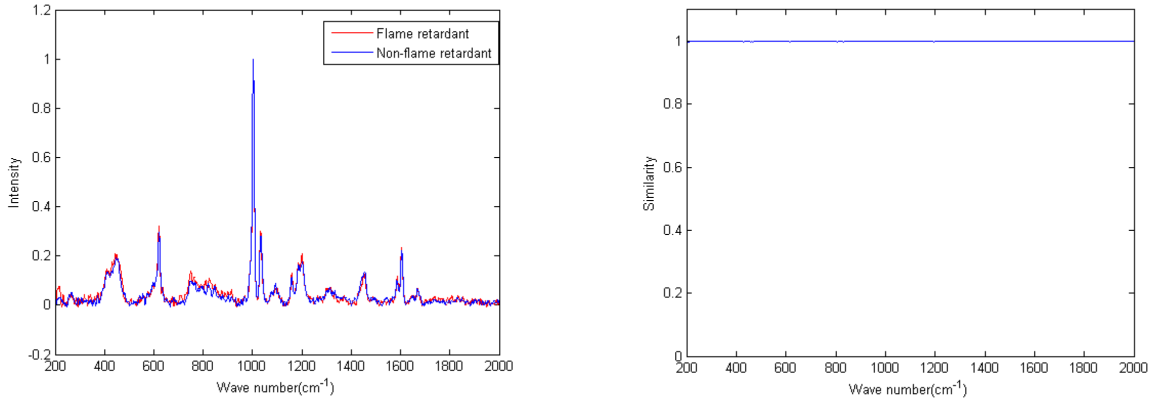

Figure 3. (a) Comparison of two tests on ABS sample without flame retardant. (b) The results obtained by moving window similarity method.

Figure 3 shows that, in all positions of the entire wave number, the similarities are close to 1. In that case we can conclude that the two spectra belong to the same sample.

4. Conclusion

This paper combines the Raman technique with similarity calculation in analysing consistency of the plastic safety parts of electrical products. As similarity calculated throughout the whole spectra from the samples of same material with different additives cannot be distinguished well, a method to use a window to scan the spectra and calculate the similarity is proposed. The experimental results show that this method can distinguish the ABS samples with and without flame retardant well, and its feasibility of this method is verified.

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