

Joint Detection and Sorting of Dangerous Chemicals Based on X-ray and Raman Spectrum

Yiying Lyu^a, Hong Min^{b*}

^aSchool of Optoelectronic Engineering, Zaozhuang University, Zaozhuang 277160, China

^bCollege of Mechanical and Electrical Engineering, Zaozhuang University, Zaozhuang 277160, China
 zhitu2010@126.com

Based on the traditional sorting methods of logistics, this paper presents a joint detection and sorting method for dangerous chemicals based on X-ray and Raman spectrum. First, the traditional wavelet transform method is improved to obtain a shift-invariant wavelet signal noise reduction algorithm, and the improved wavelet noise reduction method is applied to the Raman spectrum signal noise reduction of dangerous chemicals. The validity of the proposed method is verified with Raman spectrum analysis of ethanol and potassium nitrate. A new type of logistics sorting system is designed. The X-ray and Raman spectrum are used for the primary and secondary detection of dangerous goods respectively, and the composition of dangerous chemicals is determined by comparing the diffraction peak of the detected goods with the diffraction peak of standard chemical functional group. The designed dangerous chemicals sorting system can effectively reduce the transportation risk of dangerous chemicals. The research conclusions can provide theoretical reference for rapid sorting of storage and safe transportation of logistics.

1. Introduction

With the explosive development of e-commerce platforms (B2C, C2C, O2O, etc.), the scale of logistics industry also shows a significant trend of expansion. At the same time, express safety accidents occur more and more frequently. Once the dangerous chemicals in the logistics goods such as alcohol, explosives, drugs, and gasoline burn or explode, there will be severe casualties and economic losses (Leroux et al., 2013). In order to prevent these phenomena, the detection of dangerous chemicals and the accurate sorting of common goods and dangerous chemicals must be carried out at the source (cargo warehouse center). It is of great practical significance to study the safe and efficient detection method of dangerous chemicals and design the accurate sorting system of warehouse center for reducing logistics risk and improving logistics benefit.

Currently, the mainstream detection method of dangerous goods is to use X-rays to irradiate the goods, and to distinguish whether the goods belong to contraband products according to different colors fed back (Kolkoori et al, 2013). However, the X-ray method can only detect the general shape of the goods, but cannot determine the specific type and name of dangerous goods. For the new type of dangerous chemicals such as liquid and dust, the detection accuracy is low (Wang et al., 2018; Callerame, 2006; Kolkoori et al, 2015).

Raman spectrum has the advantages such as high resolution and low energy consumption, so it can distinguish the shape, structure and sample characteristics of goods directly by non-contact detection when applied to the safety detection of dangerous chemicals. It is a very good supplement to traditional X-ray detection, but it is still rare to jointly use X-ray and Raman spectrum to detect dangerous chemicals (Das and Agrawal, 2011).

The statistical results show that the dangerous chemicals sorting most used by logistics companies is a semi-automatic sorting system based on X-ray detection, which is not only low in detection efficiency, but also requires manual assistance in the sorting process. In this paper, based on the traditional sorting system, a method of joint detection and sorting of dangerous chemicals based on X-ray and Raman spectrum is proposed. Firstly, X-ray method is used to detect all goods quickly. When suspicious goods are detected, the intelligent sorting system is used to sort suspicious goods into the Raman spectrum detection center for

secondary detection, so as to reduce the transportation risk of dangerous chemicals. The conclusion can provide theoretical reference for fast sorting of storage and safe transportation of logistics.

2. Joint Detection of Dangerous Chemicals Based on X-ray and Raman Spectrum

2.1 One-time rapid detection technology

Using X-ray for a rapid inspection of logistics goods. When the X-ray is irradiated on the goods, some energy of the X-ray is absorbed by the goods, the X-ray direction is also changed, and then the X-ray is attenuated. Set the thickness of the goods as dx , the initial intensity of X-ray is L_x , and the intensity after irradiation is L_{x+dx} , then

$$\frac{L_x - L_{x+dx}}{L_x} = \frac{dL_x}{L_x} = -\mu dx \tag{1}$$

Assuming that the variation range of the goods thickness is $0-H$ and the variation range of the X-ray energy intensity is L_0-L_H , the Formula 1 is integrated as

$$\int_{L_0}^{L_H} \frac{dL_x}{L_x} = -\mu \int_0^H dx \tag{2}$$

A further transformation of that above Formula is carried out as

$$\ln \frac{L_H}{L_0} = -\mu H \tag{3}$$

Formula 3 is a mathematical expression of the attenuation law of X-rays. When X is irradiated to the goods, the X-ray attenuation results are different for goods with different thickness and shape, and the image of the corresponding color appears in the feedback cross section. If the color corresponding to the explosive is orange, the color corresponding to the heavy metal inorganic material is blue, and the mixture of organic and inorganic substances is detected as green.

2.2 Secondary detection technology based on Raman spectrum

In this paper, Raman spectrum is used to for secondary detection of suspicious goods. The basic detection principle of Raman spectrum is shown in Figure 1. When the incident light impinges on the detected goods, Raman and Rayleigh scattering occurs, and the structure features of the goods are exhibited by the shift of the intensity and frequency of the Raman disc.

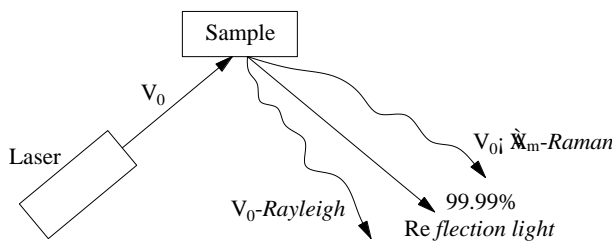


Figure 1: Basic detection principle of Raman spectrum

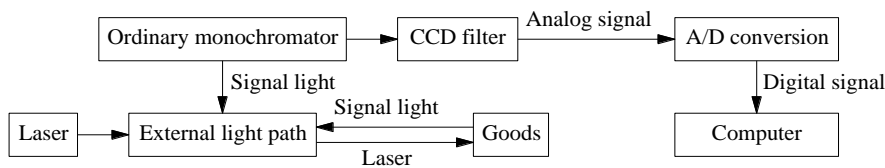


Figure 2: Structure diagram of detection system of Raman spectrometer

Figure 2 shows the detection system of the Raman spectrometer. Its laser is irradiated to the surface of the goods to analyze the chemical structure of the suspected dangerous goods or the chemical composition and concentration of the liquid goods, the collected signals are directed to the computer to complete the final confirmation.

There is a large amount of environmental noise in the signal collected in the actual monitoring. In order to remove noise from the signals, the traditional noise reduction methods mostly use wavelet transform to remove noise from the signal. Let the collected signal as

$$g(t) = f(t) + n(t) \quad (4)$$

$f(t)$ and $n(t)$ are the collected original and noise signals, respectively, and $f(t)$ is discretely sampled for wavelet transform as

$$W_s(j, k) = 2^{-j/2} \sum_{n=0}^{N-1} f(n) \psi(2^{-j}n - k) \quad (5)$$

Wavelet recursive iteration using two-scale transformation

$$W_g(j+1, k) = S(j, k) * f(j, k) \quad (6)$$

$$S_g(j+1, k) = S_g(j, k) * h(j, k) \quad (7)$$

The transformed wavelet is filtered, and the noise signal is removed and reconstructed as

$$S_g(j-1, k) = S_g(j, k) * h(j, k) + W_g(j, k) * f(j, k) \quad (8)$$

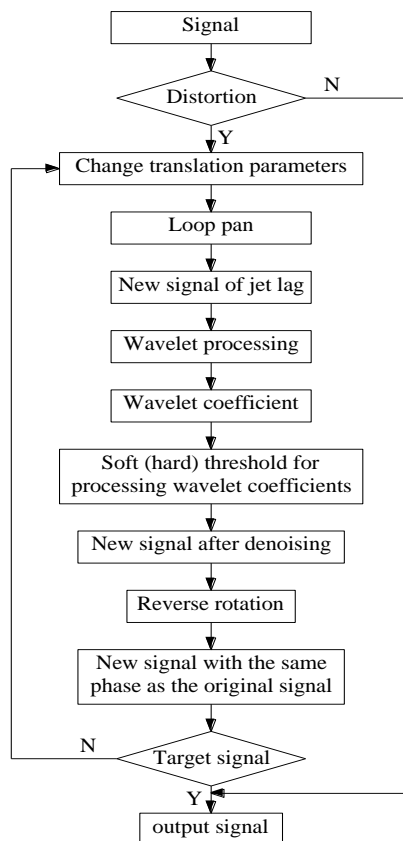


Figure 3: Improved wavelet de-noising procedures

The above-mentioned wavelet transform method uses the hard threshold to eliminate the noise signal, which often results in part of the useful signals being eliminated at the same time. In this paper, we improve the traditional wavelet transform and introduce the translation operator S^m

$$S^m(g(n)) = g((n+m) \bmod N) \quad (9)$$

Set T as the transform function of wavelet de-noising, the wavelet de-noising process considering S^m can be expressed as

$$X = S^{-m}(T(S^m(x))) \quad (10)$$

Perform multiple cyclic shifts to the signal, and after each shift, perform noise reduction processing, and accumulate the obtained results

$$X = \text{Avg}^h e^H S^{-m}(T(S^m(x))) \quad (11)$$

In summary, the improved wavelet noise reduction step proposed in this paper is shown in Figure 3.

Liquid alcohol and powdered potassium nitrate are selected as examples for detection. Alcohol and potassium nitrate are two typical dangerous chemicals, and X-rays cannot directly detect two dangerous chemicals.

Figures 4 and 5 are Raman spectrum detection results of alcohol and potassium nitrate, respectively, in which Figures 4 (a) and 5 (a) are noise-reduced by using a conventional wavelet transform. Figures 4 (b) and 5 (b) illustrate the use of the improved wavelet noise reduction method presented herein for signal noise reduction.

Comparing Figures 4 and 5, it can be seen that the improved wavelet noise reduction method proposed in this paper can effectively remove the high-frequency noise in the signal, the signal burr is significantly reduced, and the peak value corresponding to the dangerous chemicals detected in the Raman spectrum is more obvious.

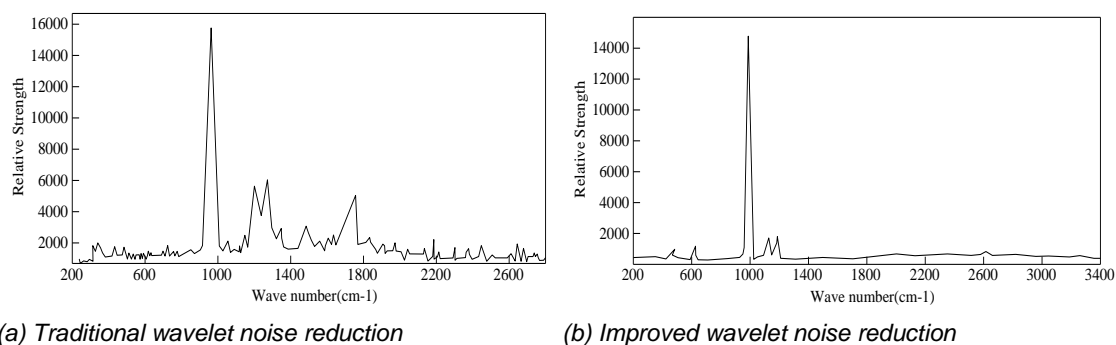


Figure 4: Two wavelet noise reduction methods for Raman spectrum noise reduction of alcohol

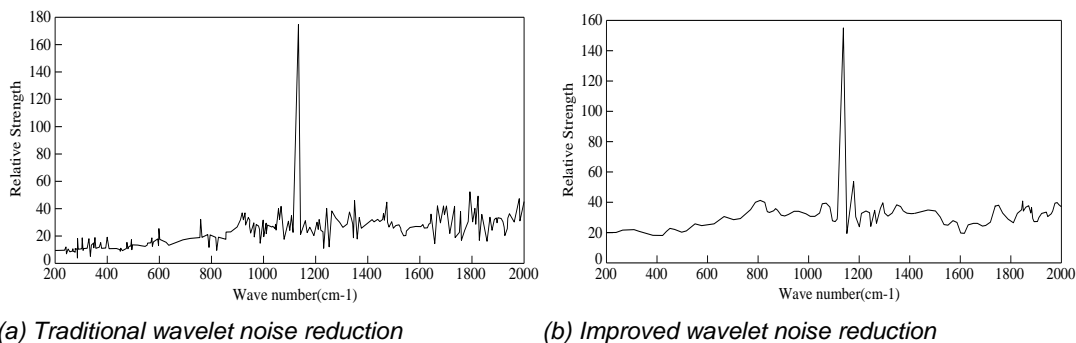
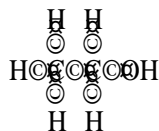
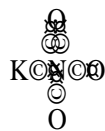


Figure 5: Raman spectrum noise reduction of potassium nitrate by two wavelet noise reduction methods

The chemical structure of alcohol and potassium nitrate is shown in Figure 6.



(a) Alcohol



(b) Potassium nitrate

Figure 6: Chemical structural formula of alcohol and potassium nitrate

Referring to Figures 4-6, it can be seen that the -C-C- group in the alcohol is in a rocking vibration state at 880/cm, and a peak of a certain scale is formed in the feedback of the Raman spectrum; near 1030/cm is the vibration peak caused by rocking vibration of -CH₂- group; in the vicinity of 1100/cm, M-type peaks of C-H-O appear, and these diffraction peaks all prove that the detected dangerous chemicals are alcohol.

In the Raman spectrum of potassium nitrate, 1036/cm corresponds to the stretching vibration peak of -NO₃, and at 1150/cm is the antisymmetric vibration peak between K and -NO₃. The diffraction peak above can prove that the detected substance is potassium nitrate.

3. Logistics Sorting System Based on Joint Detection of X-ray and Raman Spectrum

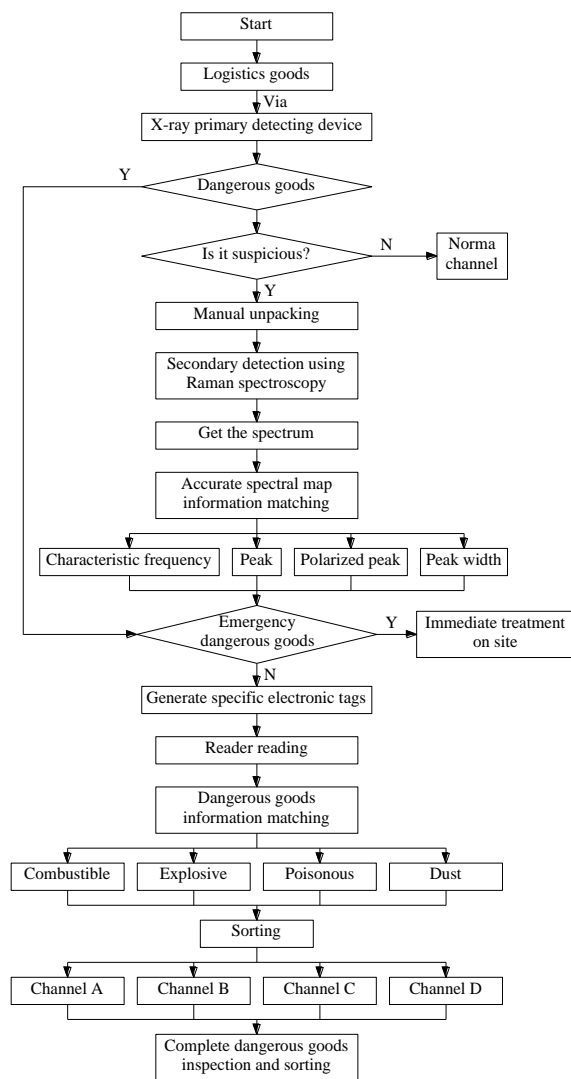


Figure 7: Logistics sorting process based on joint detection of X-ray and Raman spectrum

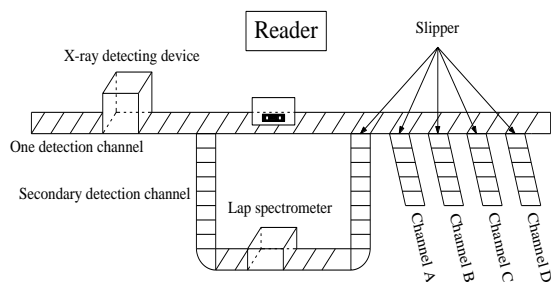


Figure 8: Logistics sorting transportation route schematic diagram based on joint detection of X-ray and Raman spectrum

According to the established joint detection of X-ray and Raman spectrum for dangerous chemicals, a logistics sorting system is constructed as shown in Figure 7. The actual goods sorting system designed is shown in Figure 8. When the goods in storage enter the sorting transportation line, they first pass through the X-ray quick detection channel to confirm the safety of most goods with obvious appearance characteristics. For goods that cannot be confirmed immediately by X-ray, they are transported to the secondary detection channel of Raman spectrum for the secondary detection by Raman spectrum. The composition of the dangerous chemicals is determined by comparing the diffraction peak of the detected goods with the diffraction peak of standard chemical functional group.

For suspicious dangerous chemicals, manual unpacking shall be carried out with final confirmation. If the test result is non-dangerous goods, the secondary package shall be carried out and then they shall be put into the transportation line. If the result of the secondary detection is dangerous chemical, the system will alarm immediately, and the personnel shall confirm the unpacking, and register the dangerous chemicals and match them with the database.

4. Conclusions

Based on the traditional sorting methods of logistics, this paper presents a joint detection and sorting method for dangerous chemicals based on X-ray and Raman spectrum. First, the traditional wavelet transform method is improved to obtain a shift-invariant wavelet signal noise reduction algorithm, and the improved wavelet noise reduction method is applied to the Raman spectrum signal noise reduction of dangerous chemicals. The validity of the proposed method is verified with Raman spectrum analysis of ethanol and potassium nitrate.

A logistics sorting system based on X-ray and Raman spectrum is designed. The X-ray is used for the primary quick detection of all goods. When suspicious goods are detected, the intelligent sorting system is used to sort the suspicious goods to the Raman spectrum center for secondary detection. The composition of the dangerous chemical is determined by comparing the diffraction peak of the detected goods with that of standard chemical functional group. The designed dangerous chemicals sorting system can effectively reduce the transportation risk of dangerous chemicals. The research conclusions can provide theoretical reference for rapid sorting of storage and safe transportation of logistics.

Reference

- Callerame J., 2006, X-ray backscatter imaging: photography through barriers, *Powder Diffraction*, 21(2), 132-135, DOI: 10.1154/1.2204054
- Das R. S., Agrawal Y. K., 2011, Raman spectroscopy: recent advancements, techniques and applications, *Vibrational Spectroscopy*, 57(2), 163-176, DOI: 10.1016/j.vibspec.2011.08.003
- Kaufman L., 2011, An evaluation of airport x-ray backscatter units based on image characteristics, *Journal of Transportation Security*, 4(1), 73-94. DOI: 10.1007/s12198-010-0059-7
- Kolkoori S., Wrobel N., Osterloh K., Zscherpel U., Ewert U., 2013, Novel x-ray backscatter technique for detection of dangerous materials: application to aviation and port security, *Journal of Instrumentation*, 8(8), 1-17, DOI: 10.1088/1748-0221/8/09/p09017
- Leroux M. H., Marcellis-Warin N. D., Trä©Panier M., 2013, Safety management in hazardous materials logistics, *Transportation Letters*, 2(1), 13-25, DOI: 10.3328/tl.2010.02.01.13-25
- Wang Y., Wu G., Yang O., Cen H., Zou B., Chen C., Lin S., Pang G., Wang Z., 2018, Design and implementation of the management and detection system of dangerous production raw materials based on odor sensor technology, *Chemical Engineering Transactions*, 68, 349-354, DOI: 10.3303/CET1868059