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Application of Principal Component Analysis in Non-Destructive Analysis

Hee-Jung Im, Byung Chul Song, Yong-Joon Park, Kyuseok Song, Won Ho Kim, Kwang Yong Jee

Nuclear Chemistry Research Division, Korea Atomic Energy Research Institute, 150, Deokjin-dong, Yuseong-gu, Daejeon 305-353,Korea, imhj@kaeri.re.kr

1. Introduction

Detection of illicit materials is achieved based on elemental compositions. Not only fissile materials [1,2] but also trace elements which have large cross sections and light elements [3,4], can be determined using the prompt gamma-ray neutron activation analysis (PGNAA) method. In PGNAA, the excited nuclei caused by an irradiation of the neutrons emit characteristic gamma rays of the object's elements, and the elemental signals are collected by detector arrays. The collected gamma spectra are applied to a principal component analysis (PCA) [5,6] to increase the signal-to-noise ratio and then to discriminate the illicit materials from the innocuous materials. The PCA results and the high penetration ability of the neutron and gamma rays contribute to reducing the probability of a false alarm for the determination of the presence of illicit materials.

2. Experimental

The experimental prompt gamma spectra were collected by using the PGNAA facility of the HANARO research reactor [3,4] (neutron fluence rate of about 1.4 $\times$ 10^8 $cm^{-2}s^{-1}$).

As samples, melamine (101.81 mg; MEL, $C_3H_6N_6$, Aldrich, 99%), potassium chloride (98.85 mg; KCl, Shynyo, 99%), polyethylene (100.07 mg; PE, $(-C_2H_4-)_n$, Aldrich), cellulose (100.81 mg; Cell, $(-C_6H_{10}O_5-)_n$), 1-(2-pyridylazo)-2 naphtol (79.09 mg; PAN, $C_{15}H_{11}N_3O$, J. T. Baker), Urea (100.05 mg; CH_4N_2O, Merck), sulfur powder (100.64 mg; S, Aldrich, 99.98%), di-phosphorpentoxid (101.03 mg; P, P_2O_5, Merck), poly vinyl chloride (98.32 mg; PVC, C_2H_3Cl), acrylic (71.95 mg; ACR, $C_{12}H_{12}N_4$), and nylon (75.05 mg; Nyl, $C_{11}H_{26}N_2O_4$), were used as non-explosive substances, but they contained similar relative concentrations of carbon, hydrogen and nitrogen as in explosives. Nitrobenzene (107.88 mg; NB, $C_6H_5NO_2$, Osaka, 99%), 4-nitrophenol (101.93 mg; NP, $C_6H_5NO_3$, Fluka, 97%), triethyl phosphate (121.36 mg; TP, $C_6H_{15}O_4P$, Yakuri, 99%), and aminobenzoic acid (101.55 mg; ABA, $C_7H_7NO_2$, Fisher), were used as explosive substances or isomers of them. Explosive imitators of ethylene glycol dinitrate (100.07 mg; EGDN, $C_2H_4N_2O_6$) and pentaerythritol tetranitrate (99.21 mg; PETN, $C_5H_8N_4O_{12}$) were prepared from a mixture of PE, $NaNO_2$, $NaNO_3$ and $NaCO_3$ for reproducing the same relative concentrations of carbon, hydrogen, nitrogen, and oxygen as in the real ones. Non-explosive sample A (99.79 mg; $C_3H_6N_3O_6$) was also prepared with the same method adopted for the imitators.

Each sample and a blank (an empty Teflon vial) were irradiated for 1000 s.

The PCA was performed by using the software package MATLAB 7.0.4 (Release 14, The MathWorks) installed in a personal computer with a Pentium V Intel processor. At first, the gamma spectra obtained from the PGNAA facilities were converted into ASCII files, and then they were imported to MATLAB to investigate the noise reduction and pattern recognition by using the PCA. Particularly nitrogen peaks (at 5269.2, and 5297.8 keV) were enlarged to discuss a noise reduction in this paper.

3. Results and Discussion

History data for the PCA were prepared from the spectra of 19 samples (MEL, KCl, PE, CEll, PAN, UREA, S, P, PVC, ACR, Nylon, NB, NP, TP, ABA, EGDN, PETN, sample A, and blank) measured each for 1000 s, and three principal components were chosen as the optimum in this case.

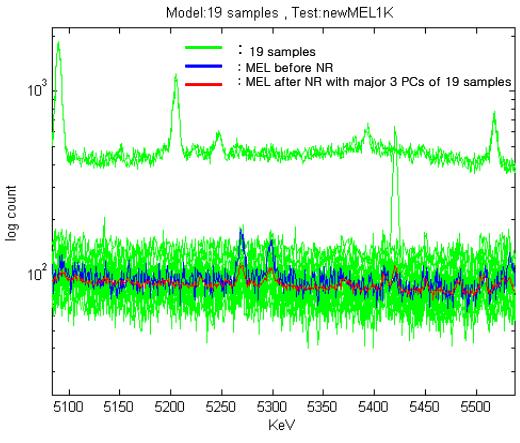

Figure 1. Projection of the MEL spectrum measured for 1000s onto the first three eigenvectors of the history data of 19 sample spectra measured each for 1000 s.

In Fig.1, the projections of a MEL spectrum measured for 1000 s onto the first three eigenvectors of the history data produced spectra, in which not only noise but also peak intensities were reduced after a reconstruction for

a noise reduction. In the case, S/N ratio increase was not significant. However, the relevant information was preserved in that the MEL spectrum maintained its individual characteristic N peaks (i.e. at 5269.2 and 5297.8 keV).

On the other hand, for a projection of a MEL data measured for 20 s onto the first three eigenvectors of the history data and then reconstruction of the spectrum (Fig. 2), an S/N ratio enhancement was observed from the non-detectable noisy raw spectrum, and the characteristic peaks were estimated by implementing PCA for the non-detectable noisy raw spectrum.

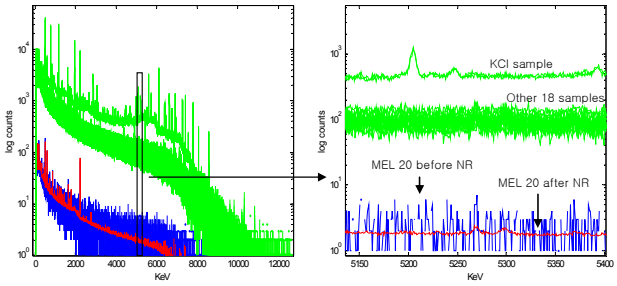

Figure 2. Projection of the MEL spectrum measured for 20 s onto the first three eigenvectors of the history data of 19 sample spectra measured each for 1000 s.

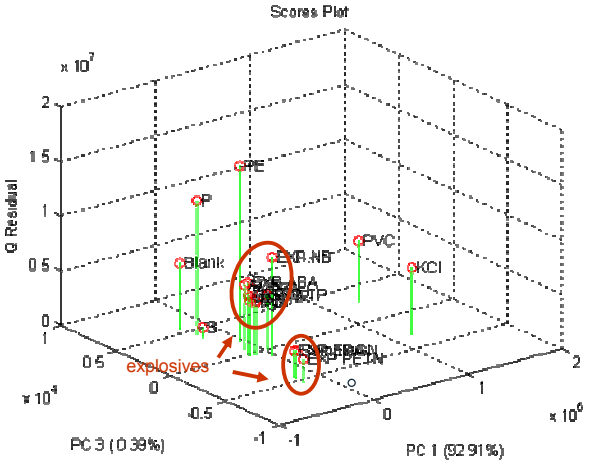

Figure 3. Pattern recognition analysis by PCA for the experimental prompt gamma-ray spectra.

After the noise reduction of spectra obtained at a very short measurement time, the spectra were applied to pattern recognition for the determination of the presence of illicit materials. The PCA results of the pattern recognition obtained using the simulated MCNP and doing experiments (Fig. 3) as data sets provided reasonable separations of the illicit materials from the innocuous materials [7].

4. Conclusion

Detection of illicit materials can be usually achieved based on certain parameters such as the geometry, vapor emissions and elemental compositions of the samples of interest. Among them, we adopted the approach of elemental composition, which involves the detection of major constituents of explosives such as N, O, C, H and Cl. We especially applied principal component analysis (PCA) to the gamma spectra obtained from the PGNAA with the effort of noise reduction and pattern recognition, compared to other nuclear based techniques.

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