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Research of CdZnTe detector based portable energy

dispersive spectrometer

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Abstract A kind of excellent CdZnTe crystal has been grown in Yinnel Tech, Inc. in recent years. Based on these CdZnTe crystals and some new techniques, a portable energy-dispersive spectrometer has been constructed which has yielded good results. CdZnTe detector has a 3% relative resolution in high-energy field and can detect gamma rays at room temperature. An integrated circuit based on preamplifier and shaping amplifier chips is connected to the detector. Voltage pulses are transformed into digital signals in MCA (multichannel analyzer) and are then transmitted to computer via USB bus. Data process algorithms are improved in this spectrometer. Fast Fourier transform (FFT) and numerical differentiation (ND) are used in energy peak's searching program. Sampling-based correction technique is used in X-ray energy calibration. Modified Gaussian-Newton algorithm is a classical method to solve nonlinear curve fitting problems, and it is used to compute absolute intensity of each detected characteristic line. **Key words** CdZnTe detector, Preamplifier, Energy-dispersive spectrometer, Spectrum analysis

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1 Introduction

Energy-dispersive (ED) spectrometer is one of the X-ray fluorescence (XRF) analysis instruments in material analysis fields today^[1]. And with development in technologies, ED spectrometer becomes more portable and intelligent.

A portable ED spectrometer could be divided into three parts: detector, electronic circuits and software (Fig.1).

Detectors work through a process of photoionization in which the interaction between the incident X-ray photon and the active detector material produces a number of electron and hole pairs. Si-PIN detector and CdZnTe detector are commonly used in portable ED spectrometer at room temperature.

A pre-amplifier is responsible for collecting a number of charges on a feedback capacitor to produce a voltage pulse proportional to the original X-ray photon energy and a shaping amplifier filters much of the noise from the signal of interest and provides a quickly restored baseline to allow high counting rates. An MCA is used to sort the arriving pulses at its input



Fig.1 Structure of the portable ED spectrometer.

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in the same fashion so as to produce a histogram representation of the X-ray energy spectrum. The MCA with USB interface has more compatibility and a higher data transfer ratio than ever.

Like other ED spectrometers, this spectrometer incorporates PC, which is available for spectral stripping, peak identification, quantitative analysis, and a host of other useful functions.

The acquired energy spectrum is first transformed to frequency domain and high-frequency noises are filtered, and then the smoothed energy spectrum is rebuilt. Numerical differentiation method is used to search the peaks of the spectrum. Sampling-based correction calibration method uses history information of the spectrum and its current state as energy calibration. This method could gain relatively high precision without radioactivity. Modified Gaussian--Newton method has been applied to obtain precise information of characteristic energy lines.

2 CdZnTe detector

Conventional high-resolution detectors usually need liquid nitrogen cooling, so room temperature detectors such as Si-PIN detector and CdZnTe detector have been developed in the recent years.

CdZnTe detectors were first developed in the beginning of the 1990s. The compound is based on the well-known material CdTe, but now a fraction of the Cd (Z=48) content is replaced with Zn (Z=30). This yields an increase in the resistivity of the material, reducing leakage current in the detectors. Yinnel Tech. Inc.^[2] has developed a Modified Vertical Bridgman (MVB) method to grow detector-grade CdZnTe crystal, and has achieved the highest electrical resistivity in the range of $(1 \sim 3) \times 10^{11} \Omega \cdot \text{cm}$, the $\mu \tau$ (e) as high as $1.8 \times 10^{-2} \text{ cm}^2 \cdot \text{V}^{-1}$, and $\mu \tau$ (h) in the range of $3 \times 10^{-5} \text{ cm}^2 \cdot \text{V}^{-1}$, respectively.

The CdZnTe crystal used in this portable ED-spectrometer has a volume of 10 mm \times 10 mm \times 1.7 mm, leakage current of 1×10^{-10} nA at room temperature, and a high detection efficiency (Fig. 2).



Fig.2 Detection efficiency of CdZnTe detector.

CdZnTe crystal is made into detector and 2.37% (FWHM) relative resolution was achieved at 59.54 keV energy peak at room temperature. Thermal noises could be further minimized through electric cooling structure (Fig. 3), thus the Lower Limit Detection (LLD) and the resolution is better and make it possible to measure X-ray fluorescence of light elements.



Fig.3 Structure of CdZnTe detector.

3 Electronics and data acquisition

3.1 Amplifier circuits

Preamplifier and shaping amplifier chips are used in amplifier circuits of this spectrometer to gain a higher performance/volume ratio.

CR-110 is a small (Fig. 4) low noise charge sensitive preamplifier (Fig. 5) intended for use with various types of radiation detectors. CdZnTe detector's current is in the range of 1 nA, so DC-coupled configuration is used to connect the detector and the preamplifier. Here, equivalent noise of CR-110 is 2.1 keV (FWHM), and gain is 1.4 V/pC.

As shown in Fig. 6, CR-200 is a single-channel shaping amplifier, intended to be used to read out the signals from the preamplifiers.



Fig.4 Structure of CR-110.



Fig.5 Simplified equivalent circuit diagram of the CR-110.



Fig.6 Equivalent circuit diagram of the CR-200.

Adding amplification stages between the preamplifier and the shaping amplifier we can obtain a greater gain, and the amplifier stages should be AC coupled to preamplifier. The noise of the voltage amplification stages should be kept reasonably low in order to take full advantage of the low noise of the preceding preamplifier stage.

Main performances of the integrated amplifier circuits and excellent NIM amplifier circuits (ORTEC 142-pc preamplifier and ORTEC 671 spectroscopy amplifier are compared here) can be seen in Table 1.

For measurement of ²⁴¹Am energy spectrum, the integrated amplifier circuits gain relative resolution of 2.37% (Fig.7) at 55.94 keV, and that of excellent NIM amplifier system gain 1.97%, while the volume of the integrated circuits is dramatically small. If electric cooling technique is used in the CdZnTe detector to lower its leakage current, a better resolution could be expected.



Fig.7 Acquired ²⁴¹Am energy spectrum using CdZnTe detector, CR-110 and CR-200 chips.

Table 1	Main performances	of CR110-CR200 circuits and	normal preamplifier and	l amplifier circuits
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Device	CR-110	ORTEC-142PC	CR-200	ORTEC-671
Decay time constant / µs	140	50		
Rise time *	7ns	25ns	2 μ s	2 μ s
Width of output pulse / μ s **			5.7	5
Equivalent noise ***	200 rms electrons	295 rms electrons	0.17 8mV	0.175 mV
Gain range			10~10000	2.5~1500
Dimensions / mm	23×24×4.3	45×132×100	23×24×4.3	34×221×265.8

*Output pulse from 0.1% to maximum amplitude (with zero input capacity and with 1 µs shaping time); **At 1% of maximum amplitude; ***With input unconnected, and with a gain of 32, at 1 µs shaping time

3.2 Data acquisition system

Universal Serial Bus (USB) is the most widely used computer interface bus today, because of its high transfer rate, plug and play, and portability. USB interface based MCA has more compatibility and flexibility. The main structure of the mini-computer based MCA is shown in Fig. 8.



Fig.8 Structure of mini-computer based MCA.

4 Spectrum analysis

4.1 FFT-ND peak-searching algorithm

The fast Fourier transform was first discussed by Cooley and Tukey^[3]. It is a discrete Fourier transform algorithm that reduces the number of computations needed for *N*-points' sequence from $2N^2$ to $2N\log_2 N$. And numerical differentiation is the process of finding the numerical value of a derivative of a given function at a given point. Traditional peak searching algorithm uses average value smooth and five-point comparison method to gain local maxima. Here the more precise and effective FFT-ND method is introduced.

4.1.1 FFT-FIR smooth

In frequency domain, signals and background are mainly in low frequency region, while noises could distribute in the whole frequency domain. The numerical energy spectrum is first transformed into frequency domain with FFT, then a low-pass filter filters high frequencies, and smooth energy spectrum is rebuilt in the end. Original energy spectrum of ²⁴¹Am and its smoothed spectrum (smoothed by FFT-FIR method) are shown in Figs. 9 and 10, respectively.



Fig.9 Original energy spectrum of ²⁴¹Am.



Fig.10 Smoothed energy spectrum of ²⁴¹Am (80% of high frequencies noises are filtered).

4.1.2 ND peak searching algorithm

Suppose the discrete function of the smoothed energy spectrum is $P_s(i)$, for any three adjacent points (j-1), j, (j+1) and their corresponding counts $P_s(j-1)$, $P_s(j)$, $P_s(j+1)$, use quadratic polynomial curve fitting ^[4].

If the quadratic polynomial have the form

$$H_i(x) = a_i x^2 + b_i x + c_i$$

use
$$\begin{cases} H_j(j-1) = P_s(j-1) \\ H_j(j) = P_s(j) \\ H_i(j+1) = P_s(j+1) \end{cases}$$
 to solve $H_j(x)$.

According to the definition of derivative:

$$P_{j}(j) = H_{j}(j) = \lim_{h \to 0} \frac{H_{j}(j+h) - H_{j}(j-h)}{2h} + R^{2}(x)$$
$$\approx \lim_{h \to 0} \frac{H_{j}(j+h) - H_{j}(j-h)}{2h}$$

when $h \to 0$, $R^2(x) \approx 0$, where $R^2(x)$ is high-order residual of x, h is step (h = 0.1 usually).

If the following expressions are true:

$$P'_{s}(i) \to 0, \quad P'_{s}(i-1) > 0, \quad P'_{s}(i+1) < 0,$$

 $P_s(i)$ could be the local maximum in the neighborhood.

The average smooth-comparison peak searching method and FFT-ND method are used in the original energy spectrum of ²⁴¹Am respectively. Results (Figs.11 and 12) show that the FFT-ND method is more effective and precise than the traditional method.



Fig.11 Peak energy positions of ²⁴¹Am using traditional smooth and peak searching algorithm.



Fig.12 Peak energy positions of ²⁴¹Am using FFT-ND algorithm.

4.2 Sampling-based correction energy calibration

In energy calibration, a radiosource with known energies is commonly used to measure its corresponding peak energy positions, then a linear relationship between energy and peak position can be established for calibration. This method is precise but cannot be applied in portable nuclear instruments because of the radioactivity. Sampling-based correction energy calibration method has been adopted in the spectrometer to replace the radiosource ^[5].

The standard sample used to calibrate has three distinct characteristic energies: E_A , E_B , E_C , each energy has a peak position: P_A , P_B , P_C in MCA.

Here,
$$E_{\overline{BA}} = \frac{E_{B} - E_{A}}{P_{B} - P_{A}}$$
 means average energy per

channel between channel $P_{\rm A}$ and $P_{\rm B}$, and so do $E_{\overline{CB}}$,

$$E_{\overline{\mathrm{CA}}}$$
.

Let
$$E_{\overline{\text{ABC}}} = E_{\overline{\text{BA}}} \alpha + E_{\overline{\text{CB}}} \beta + E_{\overline{\text{CA}}} \gamma$$

where α , β , γ are correction indexes^[5], and $\alpha + \beta + \gamma = 1$.

We measure N sets of P_A , P_B , P_C and compute E_{BA}^i ,

$$E_{\overline{\text{CB}}}^{i}$$
, $E_{\overline{\text{CA}}}^{i}$ and $E_{\overline{\text{ABC}}}^{i}$, where $i = 1, ..., N$

$$t = \frac{\overline{E_{\overline{ABC}}^{N}} - \overline{E_{\overline{ABC}}}}{S / \sqrt{N}}$$

follows *t*-distribution, where $\overline{E_{ABC}}$ is population mean. We compute sample mean $\overline{E_{ABC}^{N}}$ and sample

variance
$$S^2 = \frac{1}{N-1} \times \sum_{i=1}^{N} \left(E_{\overline{ABC}}^i - \overline{E_{\overline{ABC}}^N} \right)^2$$
. If N is big

enough, $t = \frac{\overline{E_{ABC}^{N}} - \overline{E_{ABC}}}{S / \sqrt{N}}$ follows the normal distri-

bution.

We determine confidence level p and compute confidence interval of $\overline{E_{ABC}}$, i.e. $(\overline{E_{ABC}^N} - \lambda S)$,

$$E_{\overline{ABC}}^{N} + \lambda S$$
)

We measure the standard sample and record P_A , P_B , P_C as the No.K set of data.

We compute $E_{\overline{ABC}}^{K}$. If $E_{\overline{ABC}}^{K}$ is in the interval $(\overline{E_{\overline{ABC}}^{N}} - \lambda S, \overline{E_{\overline{ABC}}^{N}} + \lambda S)$, use $E^{*} = \overline{E_{\overline{ABC}}^{N}}\phi + E_{\overline{ABC}}^{K}\phi$ as

final energy calibration, where ϕ, φ are correction

indexes and
$$\varphi = \frac{\left|\overline{E_{ABC}^{N}} - E_{ABC}^{K}\right|}{\lambda S}$$
, $\phi + \varphi = 1$; else if not,

adjust the spectrometer.

The whole computation process is shown in Fig.13.

Suppose the spectrometer has about 2% linearity drift, set $\alpha = 0.5$, $\beta = 0.2$, $\gamma = 0.3$, $\phi = 0.65$, $\phi = 0.35$, then the confidence level is set to be 95%. Compare E^* , $E_{\rm fix}$ with $E_{\rm abs}$ (Fig.14). Here $E_{\rm abs}$ is the absolute energy calibration that calibrate the instrument with radioactive sources before every measurement, and $E_{\rm fix}$ is the fix energy calibration with which once the instrument has been calibrated, the energy calibration is fixed for any measurement.



Fig.13 Flow chart of sampling-based correction energy calibration.



Fig.14 Relative error of E^* and E_{fix} to E_{abs} .

4.3 Modified Gaussian--Newton nonlinear curve fitting algorithm

As we know, energy spectrum is made of characteristic energies (each has a Gaussian shape distribution in energy spectrum) and background counts. Modified Gaussian--Newton nonlinear least-squares fitting algorithm can figure out parameters of characteristic energies' counts.

Suppose the smooth energy spectrum function is $P_{s}(i)$

Let
$$F(i) = B_3(i) + \sum_j G_j(i)$$
,

where $B_3(i)$ is cubic polynomial function to express

background, $G_j(i) = A_j \exp(-\frac{(i-\mu_j)^2}{2\sigma^2})$ to express the Gaussian function produced by *j*th energy ray in energy spectrum, F(i) is the fitting curve function expression.

Simplify the fitting curve function to

 $F(i) = F(i; X) = F(i; x_1, x_2 \cdots x_m)$

where $X = [x_1, x_2 \cdots x_m]$ is the parameter vector.

According to observed values of $P_S(i)$, determine the parameter vector and regress the function F(i;X), which best fit the objective equation:

$$Q(X) = \sum_{i=1}^{n} (P_s(i) - F(i; X))^2 = \min_{i=1}^{n} (P_s(i) - F(i; X))^2$$

First, we use Newton method to linearize the function F(i; X) at the original value $X^{(0)}$ (obtained with FFT-ND method in section 4.1) of the parameter vector X.

Second, we define A_k as the first derivative matrix of F(i; X):

$$A_{k} = \begin{pmatrix} F_{1}(1;X) & F_{2}(1;X) & \cdots & F_{m}(1;X) \\ F_{1}(2;X) & F_{2}(2;X) & \cdots & F_{m}(2;X) \\ \cdots & \cdots & \cdots & \cdots \\ F_{1}(n;X) & F_{2}(n;X) & \cdots & F_{m}(n;X) \end{pmatrix}_{X} = X^{(k)}$$

where we use A_k to compute the Hessian matrix of

F(i; X) approximately. Thus, the Newton method has been improved to Gaussian--Newton method.

Finally, we modify the Gaussian-Newton method by introducing a positive coefficient λ_m to avoid the fluctuation of algorithmic convergence.

A brief algorithmic structure of modified Gaussian-Newton method is shown in Fig.15.

Fitting result is shown in Fig.16. Each characteristic energy count could be read while fitting curve somewhat does not fit the smoothed curve well because of the thickness of the CdZnTe crystal and the incomplete collection of positive charges.



Fig.15 Flowchart of modified Gaussian-Newton algorithm.



Fig.16 Smoothed curve and fitting curve.

5 Conclusions

New architecture of portable energy dispersive spectrometer is proposed in this article. Hardware and data-processing algorithms are updated greatly to make the spectrometer more compatible and applicable and more work should be done to improve its per-

formances.

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