Material Identification Methods in Spectral Radiography Using CdTe Semiconductor Detectors

Veronique REBUFFEL, Jean RINKEL, Guillaume BELDJOUDI, Andrea BRAMBILLA
CEA-LETI, DTBS/LDET, 17 rue des Martyrs, F38054 Grenoble Cedex, France
Contact: Veronique.rebuffel@cea.fr

Abstract. Material identification in radiography is traditionally performed by dual-energy systems, using double exposure technique or two-layers detectors. Performance of such systems results from the closeness of the materials to be discriminated, from photonic noise, and energetic discriminating power of the detector. For difficult problems such as explosive detection in luggage, conventional dual-energy radiography provides only a crude material characterization. Recently emerged semiconductors based X-ray detectors offer new capabilities in energy discrimination. They provide multi-energy data, which require new methods to be processed. This paper is proposing a new material identification method based on an experimental calibration protocol. The identification process relies on a likelihood maximization among the samples of the calibration database. This study is aiming at evaluating the gain brought by spectroscopic detectors for material discrimination.

Introduction

Radiographic imaging provides a representation of the object under examination in terms of line-integrals of the attenuation coefficient, which in case of homogeneous materials, is equal to the product of attenuation coefficient by material thickness. The energy dependence of X-ray attenuation can potentially be used to characterize materials – as long as the employed acquisition system permits to obtain this information. Conventional X-ray detectors are composed of a scintillator layer coupled to a 1D or 2D array of photodiodes; they supply the deposited energy integrated over the full energy range of the generator spectrum. An only acquisition with such detectors can scarcely allow material identification. Dual-energy techniques have been developed to go further. They consist in acquiring two measurements at two energies, generally in the photo-electric and Compton domains. In terms of system, dual-energy acquisition can be performed with energy discrimination at source level - double exposure technique, where tube voltage is switched, or at detector level, by using two-layers (also called sandwich) detectors. For both cases, the information provided for each of the two energies corresponds to the integration on the corresponding range. Dual-energy techniques have been used successfully in the past twenty years for various applications. The associated data processing method is well known, generally based on the decomposition onto a material basis, an image of atomic number Z possibly being computed from the Z of the two basis materials. Optimization of the system should be performed, particularly the voltage and filter choice for double exposure technique, layers and filter thicknesses for sandwich detectors. In terms of performance, dual-energy technique allows material characterization as long as materials to be discriminated are not too close and noise level moderate [1]. Dual-energy technique has
been proved to be efficient in medical field, especially for fat quantification and bone densitometry. A very promising application field concerns composite materials, increasingly used in various industries, such as insulation or aeronautic; dual-energy approach provides information on lack of binder and enhances the fibre structure in the radiograph. Application to food industry has been developed; the challenge is to get an image by scanning the object on line without interrupting the process flow of the factory. Single exposure technique is applied with a linear sandwich detector. This technique is particularly convenient for the inspection of objects on a conveyor belt. It is the case of waste inspection, for which the speed constraint is severe (few ms$^{-1}$ translation). The application domain where most of the efforts have been spent these last years is security, and especially explosive detection in luggage, for which existing dual energy systems based on sandwich detectors [2] provide information allowing at best the distinction between organic and inorganic materials.

Differences between radiographic and tomographic techniques are essential in terms of material identification. On a tomographic image, identification can be performed directly on a voxel or a region, though several combinations of thicknesses and materials can provide similar radiographic measure. When there are only a few of materials (case of most NDT applications), dual-energy radiography permits to estimate their relative thicknesses. Otherwise, and in case of superimposition, the only solution consists in coupling image processing and identification. The method performs an image segmentation and differentially analyzes the successive material layers. This algorithm is applied for luggage inspection [3]. To sum up, the performance of dual-energy radiographic systems depends on the number of materials, prior knowledge on their nature, their closeness, the complexity of objects superimposition, the photonic noise, and of course the acquisition system. When using dual-energy integrating detectors, the obtained accuracy allows generally the material classification in only 2 or 3 Z-classes.

Recently emerged semiconductor based X-ray imaging detectors offer new capabilities in energy discrimination or spectroscopy. When associated with dedicated data processing, they can potentially improve material characterization. This paper is aiming at presenting an identification method dedicated to systems based on such detectors, and quantifying the gain in performance due to spectral data information. First we present the principle and main characteristics of semi-conductor based detectors, and show the detector response function, get by an accurate simulation tool. Then we discuss about the nature of spectral data, and propose a multi-dimensional identification method. Results are presented, based on simulation – experimental results can be found in another paper of this conference [4].

1. Spectrometric semi-conductor based detectors

Detectors made of compound semiconductors such as CdTe and CdZnTe have shown outstanding performance for X and gamma ray spectrometry when operating at room temperature [5]. Thanks to a direct conversion from photon to charges that are collected, and to dedicated electronics, they are able to count the photons and measure their energy. Recently, thanks to the progresses in device technology, energy sensitive CdTe detectors for fast digital X-ray imaging have emerged [6][7]. These detectors combine a fast read-out electronic circuit providing high count rate capabilities, and a coarse energy resolution obtained with a finite number of counters for each detector pixel. Prototypes have been developed and their performance evaluated [8][9]. LETI has developed several prototypes of spectrometric detectors optimized for various applications. They differ in terms of pixel size, material thickness, and dedicated electronics. We detail hereafter a detector
particularly suitable for line scan mode at high photon flux (1.1). A simulation software tool has been developed to model any semiconductor detector response function (1.2).

### 1.1 Spectrometric LETI detector characteristics

LETI has developed a novel fast read-out system capable of taking high-resolution spectrometric measurements at high count rates. For each pixel, the signal is continuously digitized by a 100 MHz Analog to Digital Converter (ADC), while a FPGA controls acquisition and sets up the energy spectrum on 256 bins. The set of read-out electronic components is coupled to CdTe linear array detectors. This 16 pixels array was purchased from ACRORAD (Japan). Pixel size is 0.8 x 0.8 mm². Detector is 3 mm thick and ensures good stopping power for X-rays of up to 150 keV. The spectrometric performance was characterized under X rays at fluxes up to $2 \times 10^7$ X/mm²s. They are described in a former paper [10]; we summarized them now. Fig.1a shows the spectrum measured with a 80 keV ESRF X-ray source. Increasing the count rate leads to resolution deterioration and count loss. Up to $2 \times 10^6$ photons/pixel/s, we observed that the spectrum does not suffer particularly from pile up phenomena (Fig.1b). A dead time of 73 ns has been calculated by adjusting experimental count rates with a non-paralysable behavior model. In a typical configuration for luggage inspection ($2 \times 10^6$ photons/pixel/s without attenuating object, equivalent to $3.1 \times 10^6$ photons/mm²/s), resolution is 10% at 122 keV.

![Fig. 1. Performance of a LETI spectroscopic detector.](image)

(1a): Response to an 80 keV X-ray source at high flux. (1b): Count rate performance as a function of flux

### 1.2 Simulation of the detector response

An accurate model of a semiconductor detector response has been developed. It takes into account various physical phenomena inside the detector: matter-photons interactions (absorption, diffusion and fluorescence, modelled using a Monte-Carlo software) and electronic processes (charge collection, charge sharing, pulse pile-up, K-shell escape). The output of the software is composed of all the responses of the detector to each energy bin, sampled on the specified energy bins, this set being stored in a matrix form. An example is presented in Fig.2 for a detector geometry 0.8 x 0.8mm² x 3mm. The response matrix in imaged in Fig.2a, it would be diagonal if the detector was perfect. A vertical profile is shown in Fig.2b, it corresponds to the response at a 80 keV pulse. The tailing is non negligible, and results from charge sharing. The simulated spectrum shows a good agreement with the experiments (Fig.2c, for an X-ray spectra at 120 kV, filtration 4mm Al). This modeling software permits to predict the detector response depending on characteristics such as pixel size or detector thickness. The detector can then be optimized depending on application constraints. The simulation tool is also helpful for reducing the detector imperfections. The software has been linked to a program providing realistic
simulated radiographs, allowing the evaluation of the detector performance in terms of radiograph quality, and the validation of the developed processing methods.

Fig. 2. Simulation of a detector response.
(2a): Detector response matrix. (2b): Response at a 80 keV pulse. (2c): Comparison between simulated and experimental spectra, X-ray spectrum at 120 kV.

2. Spectral information analysis

For an incident spectrum $N_0(E)$ the expected number of transmitted photons at energy $E$ through an object of thickness $th$ of a material characterized by its linear coefficient attenuation $\mu(E)$ is:

$$N(E) = N_0(E)\exp(-th \cdot \mu(E)).$$

The “detector measurement”, information provided by the detector, depends on its type. A spectroscopic detector is able to provide a number of photons per energy bins, these bins being narrow – about 1.2 keV for our prototype – sufficiently narrow for considering the attenuation function $\mu(E)$ constant inside them. This bin information can be merged into larger channels. For $K$ channels, each of them defined by an energy range $[E_{k,\text{min}}, E_{k,\text{max}}]$, we get a vector of $K$ measurements:

$$m = (m_1, \ldots, m_k, \ldots, m_K) \text{ with } m_k = \sum_{E_{k,\text{max}}}^{E_{k,\text{min}}} N(E)$$

Notice that the thresholds are not necessarily contiguous ($E_{k,\text{max}} \leq E_{k+1,\text{min}}$). $K$ is equal to 1 for a counting mode detector, and to $nbE$ for spectroscopic detector, for which the energy channels equal the energy bins ($m_i = N(E)$). The “attenuation measurement”, which is precisely the line-integral of the attenuation coefficient, is given by the vector:

$$\text{att} = (\text{att}_1, \ldots, \text{att}_k, \ldots, \text{att}_K) \text{ with } \text{att}_k = -\log \frac{m_k}{m_{0,k}}$$

Due to the energy dependence of $\mu$ (known as beam hardening effect), this measurement is clearly non linear in material thickness, except for thin channels.

To obtain a realistic measure, the detector response has to be considered. If it is modelled by a matrix $R$, the measured number of photons $N$ should be replaced by the matrix product $R \cdot N$ in the preceding equations. The detector response induces a non linearity of the measurement even for spectroscopic detectors.

For a spectroscopic detector, the resulting data set – typically 100 values $m_i$ for a 20-120 keV spectrum, is large and may be difficult to be stored and processed, especially in tomographic mode. The use of larger channels may be preferred. Formerly the information is then similar to those produced by a multi-counting detector using electronic counters. Numerical merging of spectral data is more complex but offers capabilities such as
adaptability by tuning the channels thresholds, or detector imperfections correction before merging. Other merging functions can be implemented. For instance, instead of computing the sum of the bins information followed by the attenuation, it is possible to sum the elementary attenuations [11], making the obtained data directly linear to material thickness. In the following we consider any multi-counting or spectroscopic detector, resulting in K measurements on K channels of any width: \( \text{att} = (\text{att}_1, \ldots, \text{att}_K) \) (called attenuation vector), including the particular case where channels equal energy bins (\( K = n b E \)).

3. Material identification method for radiography

3.1 Calibration Protocol

The calibration process consists in placing in the radiographic system a previously defined set of various materials and thicknesses, and for each sample, to learn the probability distribution of the attenuation vector \( \text{att} \) using successive measurements at representative noise conditions. The number of measurements should be great enough to assure robust statistics (typically 2000 in our case). Fig.3a presents a calibration database composed of 3 materials, using a dual-counting detector (\( K = 2 \)). For comparison purpose, Fig. 3b shows the same database but with measurements acquired by a sandwich detector.

Fig. 3. Example of a calibration database using three plastic materials: PE, POM and PVDF. PE thicknesses range from 1 to 20 mm, POM and PVDF thicknesses range from 1 to 10 mm (both 1 mm steps). (3a): Ideal dual-counting detector (\( K = 2 \), channels [21-30] / [44-110] keV). (3b): Ideal sandwich detector.

For each calibration sample represented by its material and thickness (\( \text{mat}, \text{th} \)), the \( \text{att} \) distribution is modelled by a multi-normal distribution (mean values K-vector \( \text{m} \), and covariance matrix \( \Sigma \), \( \Sigma \) being diagonal is case of a spectrometric detector):

\[
 f_{\text{mat,th}}(\text{att}) = f_{\text{m,}\Sigma}(\text{att}) = \frac{1}{(2\pi)^{K/2} |\Sigma|^{1/2}} e^{-\frac{1}{2}(\text{att} - \text{m})'\Sigma^{-1}(\text{att} - \text{m})} f_{\text{mat,th}}(\text{att})
\]

The thicknesses range should cover the variation range of the examined objects, and be sufficiently sampled to allow linear interpolation of the statistics between two successive thicknesses.

3.2 Identification process

Given a current measurement represented by an attenuation vector \( \text{att} \), the probability density values corresponding to the different calibration samples \( f_{\text{mat,th}}(\text{att}) \), including those at interpolated thicknesses, are computed at the point \( \text{att} \). The values for the different materials are mutually compared, and the highest is selected, giving the more probable material \( \text{mat} \) (and incidentally the estimated thickness):

\[
 \text{mat} = \arg \max_{\text{mat}_{\text{x,database}}} f_{\text{mat}_{\text{x,th}}}(\text{att})
\]
Notice that if the examined \textit{att} is approximately at the mid-distance of two materials, it may be no meaningful to choose between both, and wiser to report the decision later on (using other measurement, other view, or merging pixels before identification). A confidence index may be defined, using the set of probability density values for the overall database. For instance we propose a normalized index, noted $L$ for likelihood, which ranges from $1/N_{\text{mat}}$ when no material distinction is possible, to 1 if the material is correctly identified:

$$L_{\text{att}} = \frac{\max_j \hat{f}_{\text{mat}_j}(\text{att})}{\sum_{j} \hat{f}_{\text{mat}_j}(\text{att})} \quad \text{with} \quad \hat{f}_{\text{mat}_j}(\text{att}) = \max_{k} f_{\text{mat}_j,k}(\text{att})$$

The global identification strategy should be defined together with the choice of the calibration database, and depends strongly on the application context. If only a few materials are concerned, if they are well-known and not dangerous, it is recommended to choose them as database representatives. Otherwise, if a connected area in the $K$-vector \textit{att} space can be defined, as it is the case for explosives detection (see next part), representatives bordering materials are correct. Other strategies may be envisaged, in terms of representativeness of database, number of database samples, and identification criteria. For system performance quantification, a binary criterion is often used. Each elementary detection process is considered as true if the selected material is correct, false elsewhere. Repeated over a large set of experiments, this process allows the statistic computation of a false detection rate. Notice that until now, the performance was quantified using one sample only. The same evaluation can be performed on different thicknesses of a given material, on different materials, or on all possible samples.

### 3.3 Optimization of detector configuration

Material identification performance is based on a trade-off between measurement noise and material distinction. For a spectrometric detector, the optimization process aims at choosing the set of energy channels that maximizes material discrimination inside the calibration database. This choice is all the more important that the channels are large.

For that optimization, some authors [12] propose a lower bound Cramer-Rao criterion. The criterion for the material thickness variance estimator has been adapted to an identification task. For this criteria being applied to an non–ideal system, it is necessary to dispose of a model of the detector response. We proposed another criterion based on statistical results of identification process [11]. Optimal configurations are very similar to those get by Cramer-Rao criteria. Our method is more time consuming, but it implicitly takes into account the system imperfections without requiring an explicit model, thanks to experimental measurements process. However, it is important to highlight the dependence of the optimization results with the choice of the sample (material nature and thickness).

Spectroscopic detectors (1keV width bins) does not require optimization.

### 4. Results

#### 4.1 Materials and System simulation

The example addresses the context of homeland security, and more precisely the explosive materials identification. The effective atomic number ($Z_{\text{eff}}$) of most explosive materials ranges from 7 to 7.8. Two inert plastics, PolyEthylene (PE) and PolyVinylDene Fluoride (PVDF) with respective $Z_{\text{eff}}$ of 5.95 and of 8.31, are chosen as their $Z_{\text{eff}}$ border the explosive $Z_{\text{eff}}$ range. A third inert plastic, the PolyOxyMethylene (POM) with a $Z_{\text{eff}}$ of 7.38 cannot be distinguished from common explosives, making it an appropriate candidate for an explosive
Materials simulator. Material thicknesses for the calibration database range from 1 to 20 mm for PE, and from 1 to 10 mm for POM and PVDF materials, both in 1 mm steps. The simulated detector is based on a CdTe architecture with a pixel 800x800 µm² sized and 3 mm thick. The spectrometric detector is 1 keV bin width. Energy ranges from 21 keV to 110 keV, which results in sampling spectra into 90 bins. In a first approach, an ideal response function of the detector is assumed. A tube voltage of 115 kV with a 3 mm Aluminum filtration is used, tuned to fit a primary beam fluence of 7.8x10⁴ photons.mm⁻².

4.2 Performance depending on channels configuration and object thickness

For a channel number K = 2 to 5, the thresholds have been optimized by maximisation of the likelihood for 3 mm of POM [11]. For K=2 the optimal channels are [21-30 keV] and [44-110 keV]. Notice the presence of a gap between the two channels, already commented in literature [12]. For K=3 we get [21-26 keV], [26-34 keV] and [44-110 keV]. For K> 5, optimization is time consuming, and less required because channels become necessarily thinner. Using optimized channels for K = 2 to 5, and equally distributed over the energy range channels for K = 10 to 90, we studied the identification performance of the sample (POM, 3 mm). We used the likelihood index introduced in §3.2 evaluated statistically, here ranging from 1/3 when no identification is possible to 1 for correct identification. Fig. 4 shows that performance increases regularly with the channels number. Performance is higher for optimized channels, but this optimization is material dependant.

![Fig. 4. Performance, expressed with Likelihood index, as a function of channels number.](image)

Concerning the false detection rate (FDR), we get for instance for 4 mm of POM, FDR=18% for the optimized dual counting detector, FDR=14% for the spectroscopic detector (90 channels), to be compared to FDR=66% for a sandwich detector [11].

![Fig. 5. Example of colour imaging, for a sandwich detector and a spectroscopic one (2 & 90 channels).](image)
4.3 Colour Imaging

In order to help visual comparison, we simulated the identification process on a test object composed of the 3 database materials, with thicknesses from 3 to 8 mm (Fig.5). Resulting images for sandwich detector, dual-counting detector and spectroscopic detector (1 keV width channel) are shown. Every pixel is coloured accordingly to the estimated material. The enhanced identification capability of the spectrometric detector compared to the dual-counting one and even more to the sandwich one can be deduced visually by the reduction of colour mixing for each insert.

Conclusion

A new material identification method has been proposed to process projection data acquired by any spectroscopic detector. It has been tested by simulation using an ideal spectrometric detector, illustrating clearly the interest of a large number of channels. When using the spectral method (1 keV width channels) the results show a significant decrease of false detection rate compared to an optimized dual counting approach applied on the same spectrometric raw data. Compared to a sandwich detector, the false detection rate is decreasing by a factor higher than 3. Generally, our study demonstrates the performance and robustness continuous increase with the number of detector energy channels. A software tool has been developed for modeling the response of a spectroscopic detector, in order to model non perfect detectors. Experimental preliminary results can be found in [13]. Future works will concern object superimposition in radiography.

References